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Volume 1: User's Guide

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THE HYDROCARBON SPILL SCREENING MODEL (HSSM)
VOLUME 1: USER'S GUIDE

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Disclaimer

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All research projects making conclusions or recommendations based on environmentally related measurements and funded by the United States Environmental Protection Agency are required to participate in the Agency Quality Assurance Program. This project did not involve environmentally related measurements and did not involve a Quality Assurance Plan.

The computer program described within this report simulates the behavior of water-immiscible contaminants (NAPLs: NonAqueous Phase Liquids) in idealized subsurface systems. The approaches described are not suited for application to heterogeneous geological formations, nor are they applicable to any other scenario other than that described herein. The model is intended to provide order-of-magnitude estimates of contamination levels only. The full model has not been verified by comparison with either lab or field studies. Therefore the EPA does not endorse the use of this computer program for any specific purpose. As in the case of any subsurface investigation, the scientific and engineering judgement of the model user is of paramount importance. Any model results should be subjected to thorough analysis. In this user's guide, typical values are given for various parameters. These are provided for illustrative purposes only.

When available, the software described in this document is supplied on an "as-is" basis without guarantee or warranty of any kind, expressed or implied. Neither the United States Government (United States Environmental Protection Agency, Robert S. Kerr Environmental Research Laboratory), The University of Texas at Austin, Computer Sciences Corporation, nor any of the authors accept any liability resulting from the use of this code.

Foreward

EPA is charged by Congress to protect the Nation's land, air and water systems. Under a mandate of national environmental laws focused on air and water quality, solid waste management and the control of toxic substances, pesticides, noise and radiation, the Agency strives to formulate and implement actions which lead to a compatible balance between human activities and the ability of natural systems to support and nurture life.

The Robert S. Kerr Environmental Research Laboratory is the Agency's center of expertise for investigation of the soil and subsurface environment. Personnel at the Laboratory are responsible for management of research programs to: (a) determine the fate, transport and transformation rates of pollutants in the soil, the unsaturated and the saturated zones of the subsurface environment; (b) define the processes to be used in characterizing the soil and subsurface environments as a receptor of pollutants; (c) develop techniques for predicting the effect of pollutants on ground water, soil, and indigenous organisms; and (d) define and demonstrate the applicability of using natural processes, indigenous to the soil and subsurface environment, for the protection of this resource.

One of the most common, yet complex, class of subsurface contaminants are the light nonaqueous phase liquids (LNAPLs). Although the LNAPL itself remains distinct from the subsurface water, chemical constituents of the LNAPL can cause serious ground water contamination. Since a number of phenomena and parameters interact to determine contaminant concentrations at the receptor points, models are needed to estimate the impacts of LNAPL releases on ground water. This user's guide describes the Hydrocarbon Spill Screening Model (HSSM) which is intended to simulate release of an LNAPL. The intent of the model is to provide a practical tool which is easy to apply and runs rapidly on personal computers.

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Abstract

This user's guide describes the Hydrocarbon Spill Screening Model (HSSM). The model is intended for simulation of subsurface releases of light nonaqueous phase liquids (LNAPLs). The model consists of separate modules for LNAPL flow through the vadose zone, spreading in the capillary fringe, and transport of chemical constituents of the LNAPL in a water table aquifer. These modules are based on simplified conceptualizations of the flow and transport phenomena which were used so that the resulting model would be a practical, though approximate, tool. Both DOS and Windows interfaces are provided to create input data sets, run the model, and graph the results. These interfaces simplify the procedures for running the model so that the model user may focus on analysis of his/her problem of interest. To that end, guidance is given for selecting parameter values and several utility programs are provided to calculate certain parameters. Typical example problems, which begin with a general problem statement, show exactly how each parameter of the model should be chosen.

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List of Symbols

Latin

A	Area
a_v	Aquifer vertical dispersivity
B	Bulk partition coefficient defined by equation (25)
$B(\omega)$	Time varying function of concentration at boundary (equation (86))
b	Aquifer saturated thickness
b_o	Observation well thickness of NAPL
$\mathbf{C}$	Nondimensional concentration (equation (81))
c, c_w	Concentration of the constituent in the water phase
c_m	Maximum concentration
c_o	Concentration of the constituent in the NAPL phase
$c_{o(soil)}$	Constituent concentration in the NAPL in equilibrium with the soil
$c_{o(surf.)}$	Constituent concentration in the released NAPL
c_s	Sorbed phase concentration of the constituent
$c_{w(initial)}$	Initial water phase concentration of the constituent
c_{wo}	Equilibrium constituent concentration for water in contact with the NAPL
$\mathbf{D}$	Nondimensional dispersion coefficient (equation (81))
D_o	Formation free-product thickness
D_L	Longitudinal dispersion coefficient
D_T	Transverse horizontal dispersion coefficient
D_V	Vertical dispersion coefficient
d_{pz}	Depth of the NAPL contaminated zone
E	Constant defined by equation (93)
erf()	Error function
erfc()	Complementary error function
F_1	OILENS NAPL source head function
F_2	OILENS lens radius function
f_n	n^{th} function to be solved for a general Runge-Kutta scheme
G	Known constant that relates lens source heads and radii at different times
g	Acceleration of gravity
H	Sum of the NAPL head terms in KOPT; Total penetration depth of leachate in TSGPLUME
H_{adv}	Penetration depth due to vertical advection of water entering the aquifer
H_{dis}	Penetration depth due to vertical dispersion in the aquifer
H_f	NAPL head at the NAPL front
H_s	NAPL head at the surface
h	Pressure head in KOPT (equation (16))
h_{cao}	Air-NAPL capillary pressure head
h_{caw}	Air-water capillary pressure head
h_{cij}	Capillary pressure head or capillary rise for the i-j fluid pair
h_{ceao}	Air-NAPL entry head
h_{ceaw}	Air-water entry head
h_o	NAPL head at a given location
h_{os}	NAPL head in the lens below the source (Figure 16)
h_{ow}	NAPL-water capillary pressure head
I_d	Value of the integral in equation (56)
I_r	Rate of infiltration outside the facility
J	Advective flux
J_c	Mass flux of the chemical constituent
K	Hydraulic conductivity

K_{ei}	Effective conductivity to fluid i
K_{eo}	Effective conductivity to NAPL
K_{si}	Saturated conductivity to fluid i
K_{so}	Saturated conductivity to NAPL
K_{sw}	Saturated conductivity to water
k	Intrinsic permeability
k_d	Soil/water partition coefficient
k_i	Fluid i/water partition coefficient
k_o	NAPL/water partition coefficient
k_{ri}	Relative permeability to fluid i
k_{rw}	Relative permeability to water
k_{ro}	Relative permeability to NAPL
L	Length (in direction of ground water flow) of a surface facility
$L(y)$	Length of a chord of a circle
M_t	Total constituent mass in the NAPL lens
m_c	Mass of constituent per unit volume
m	Mass flow rate
m_{diss}	Total constituent flux into the aquifer
m_{infil}	Mass loss rate to the aquifer (equation (48))
m_{source}	Ground water source term from the NAPL lens
n	Time level
p_i	KOPT model parameter
Q_{KOPT}	KOPT-determined NAPL inflow rate (Figure 16)
Q_{loss}	Loss rate of NAPL from source cylinder (Figure 16)
Q_{out}	NAPL loss rate due to dissolution and trapping (equation (43))
Q_{radial}	Lateral flow from the source cylinder (Figure 16)
q	Darcy velocity in aquifer below facility (equation (67))
q_i	Flux of fluid i
q_o	NAPL flux
q_w	Water flux
q_{wi}	Volume flux of infiltrating rainfall
R	NAPL lens radius
R_d	Retardation factor
R_s	NAPL source radius
R_t	Lens radius
r	Radius
S_{ar}	Residual air saturation
S_i	Saturation of fluid i
S_{ir}	Residual saturation of fluid i
S_o	NAPL saturation
$S_{o(max)}$	Maximum NAPL saturation in KOPT solution
S_{or}	Residual NAPL saturation
S_w	Water saturation
$S_{w(avg)}$	Water saturation associated with the average annual recharge rate
S_{wr}	Residual water saturation
SC_i	First order sensitivity coefficient for the KOPT model
$\mathbf{T}$	Nondimensional time (equation (81))
t	Time
t_o	Time origin
V_C	Volume of source cylinder beneath the surface source (equation (90))
V_L	NAPL volume in the spreading lens
V_o	NAPL volume incorporated into the soil in KOPT
V_T	Total lens volume (including LNAPL, water and soil)
V_{vz}	Total lens volume (including LNAPL, water and soil) in the vadose zone

V_{sz}	Total lens volume (including LNAPL, water and soil) in the saturated zone
v	Seepage velocity in the aquifer
W	Width (across the direction of ground water flow) of a surface facility
w	Variable of integration in equations (55) and (95)
w_R, w_{Rs}	Limits of integration in equation (95)
X	Nondimensional x coordinate (equation (81))
x	Distance from upgradient edge of NAPL lens
Y	Nondimensional y coordinate (equation (81))
$y_1, y_2, ..., y_n$	1st through nth independent variable
Z	Nondimensional z coordinate (equation (81))
z	Depth
z_{ao}	Level of the air-NAPL interface
z_{aw}	Level of the air-water interface (water table) in the absence of NAPL
z_{ow}	Level of the NAPL-water interface
z_f	Front depth in KOPT

Greek

β	Density term in equation (36)
ΔM_L	Constituent mass loss from NAPL lens during a time step
ΔV_L	Volume of free product (LNAPL) that becomes trapped in a time step
ΔV_R	Change in total lens volume (LNAPL, water and soil)
$\delta m(y)$	Increment of mass flux into the aquifer
ϵ	Brooks and Corey relative permeability exponent
η	Porosity
Λ	Nondimensional effective decay coefficient in TSGPLUME (equation (81))
λ	Brooks and Corey capillary pressure exponent; Decay coefficient in TSGPLUME
λ^*	Effective decay coefficient in TSGPLUME
μ_i	Dynamic viscosity of fluid i
μ_o	Dynamic viscosity of the NAPL
ρ_b	Bulk density
ρ_i	Density of fluid i
ρ_o	Density of NAPL
ρ_w	Density of water
σ	Standard deviation
σ_{aw}	Water surface tension
σ_o, σ_{ao}	NAPL surface tension
σ_{ow}	NAPL-water interfacial tension
θ_o	Volumetric NAPL content
θ_{orv}	Volumetric residual NAPL content in the vadose zone
θ_{ors}	Volumetric residual NAPL content in the aquifer

List of Abbreviations and Acronyms

CSMoS	Center for Subsurface Modeling Support
HSSM	Hydrocarbon Spill Screening Model
HSSM-KO	Computer code that implements KOPT and OILENS
HSSM-T	Computer code that implements TSGPLUME
KOPT	Kinematic Oily Pollutant Transport (vadose zone portion of HSSM)
LNAPL	Lighter-that-water nonaqueous phase liquid
NAPL	Nonaqueous phase liquid
OILENS	HSSM Module for NAPL lens motion and chemical dissolution into the aquifer
RSKERL	Robert S. Kerr Environmental Research Laboratory
TSGPLUME	Transient source gaussian plume model (aquifer module of HSSM)
USEPA	United States Environmental Protection Agency

Acknowledgment

The authors express their appreciation to Susan Roberts-Shultz for the original development of OILENS, to Mike Johnson for the original development of TSGPLUME, to Donald Collings for developing the DOS preprocessor, to Mark Lee for developing the REBUILD and DOS menu programs, to Julia Mead and Sarah Hendrickson for repeated testing of HSSM test data sets; and to Dr. Jeffrey A. Johnson, Dr. Varadhan Ravi and Rick Bowers for extensive beta testing.

Section 1 Introduction

When fluids that are immiscible with water (the so-called nonaqueous phase liquids or NAPLs) are released in the subsurface, they remain distinct fluids, flowing separately from the water phase. Fluids less dense than water (LNAPLs) migrate downward through the vadose zone, but upon reaching the water table, tend to form lenses on top of the aquifer. Generally, the fluids are composed of complex mixtures of individual chemicals, so that aquifer contamination results from the dissolution of various constituents of the LNAPL. This document describes a screening model called the Hydrocarbon Spill Screening Model (HSSM) for estimating the impacts of this type of pollutant on water table aquifers. The model is based on approximate treatments of flow through the vadose zone, LNAPL spreading along the water table, and miscible transport of a single chemical constituent of the LNAPL through a water table aquifer to various receptor points. Emergency response, initial phases of site investigation, facilities siting, and underground storage tank programs are potential areas for use of HSSM.

The user's guide is organized into sections that describe the assumptions underlying the model, the required input data and the mechanics of running the model. Separate MS-DOS and MS-Windows interfaces are provided for the model. Each interface has the capability to enter and edit input data sets, run the model, and display graphs of the results. The advantages and disadvantages of each interface are briefly described in order to aid the user in selecting the appropriate interface for his/her hardware and software configuration. Following the description of the interfaces, several example problems are presented that illustrate the steps necessary for setting up and running the model.

1.1   The Meaning of the Name HSSM

Each word in the name of the model is used below as a point-of-departure for a discussion of some issues related to use of the model. Specific information on the model's parameter values and directions for use of the model are given in later sections.

1.1.1 Hydrocarbon

In HSSM, the LNAPL (or *hydrocarbon*) is assumed to be composed of two components. The first component is the LNAPL itself, which is a liquid that is separate from and does not mix with the subsurface water. The model contains a set of equations for tracking the motion of the LNAPL phase. Several of the results and graphs produced by the model depict the distribution of the LNAPL phase. The second component is referred to as a *chemical constituent* of the LNAPL, because typical LNAPLs are composed of many individual chemicals. HSSM tracks the transport of one of these chemicals. Since the chemical constituent may dissolve into the subsurface water, it can be transported by the groundwater and contaminate down gradient receptor points. For example, HSSM may be used to simulate a gasoline release. Benzene could be the chemical constituent of interest. All of the rest of the chemicals composing the gasoline would be treated as being part of the LNAPL. When the impact of another constituent of gasoline, say toluene, needed to be determined, the chemical constituent would be the toluene. In this way, HSSM could be run for several of the important chemical constituents of the LNAPL. The model user could develop a feel for the behavior of the different chemicals by comparing the results.

HSSM is designed for LNAPLs. It is not suitable for denser-than-water NAPLs (DNAPLs) as the NAPL is assumed to "float" on the water table. The vadose zone module of HSSM (Section 2.1) could, however, be used for a DNAPL, as the qualitative behavior of that module is not affected by fluid density.

1.1.2 Spill

Spill is used as a generic term for a release of LNAPL. The release may be a spill, leak or other event which allows the LNAPL to enter the subsurface. In HSSM some details of the release must be known as they are required for input to the model. These details may include the beginning and ending times of the release, the rate of release of the LNAPL or the ponding depth of the LNAPL at the surface.

1.1.3 Screening Model

Screening models may include a variety of chemical and hydrological processes, but usually do not include subsurface heterogeneity. Most screening models are in the form of analytical solutions of their governing equations. Simplifications must usually be made in order to get these analytical solutions. As a result, computer implementations of screening models use only relatively small amounts of computer time. In general, screening models can be used to estimate the impacts of contamination, given their assumptions. The HSSM is a screening model; it includes a number of chemical and hydrologic phenomena, assumes subsurface homogeneity, executes rapidly on PCs, and excludes some phenomena. For example, if gasoline is spilled, HSSM may be used to give a rough estimate of ground water concentrations of constituents of the gasoline. The model is intended only to give order-of-magnitude results, because a number of potentially important processes are treated in the model in an approximate manner or are ignored entirely. Also, one would not expect to calibrate the model by adjusting the spatial distributions of the parameters, as heterogeneity is not included in the model.

If simulation of complex heterogeneous sites is needed or other approximations made in HSSM are unacceptable, then a more inclusive model, such as the MOFAT code developed at Virginia Polytechnic Institute (Kuppusamy et al., 1987); the SWANFLOW code developed by Geotrans, Inc. (Faust, 1985); the MAGNUS code developed by Hydrogeologic, Inc. (Huyakorn and Kool, 1992); or the VALOR code developed by The Electric Power Research Institute (Abriola et al., 1992) should be used instead of, or in addition to, HSSM. Potential users of HSSM should pay close attention to the following discussion of the assumptions and limitations of the model, so that they may make an informed decision on the use of the model.

1.2 Components of the Model

Figure 1 shows a typical release of a LNAPL pollutant at the ground surface. The LNAPL flows downward through the vadose zone due to gravity and capillary forces. The LNAPL is deflected from its downward path by geologic heterogeneities it encounters on its way toward the water table. Infiltrating rainwater may push the LNAPL down faster than it would move on its own. Once in the vicinity of the water table, the LNAPL floats in the capillary fringe since it is a nonwetting phase that is less dense than water. Fluctuation of the water table due to natural causes or wells may create a smear zone containing trapped LNAPL. Contact with the ground water or infiltrating recharge water causes the chemical constituents of the LNAPL to dissolve, resulting in aquifer contamination. The constituents may be leached at different rates due to their diverse properties. Depending on their volatility, the constituents also partition into the vadose zone air.

Once in the aquifer, limited mixing leaves the constituents in a relatively narrow band near the top of the aquifer. These constituents are transported by advection and dispersion through the aquifer. The aquifer, like the vadose zone, is heterogeneous and flow may follow preferential pathways.

The HSSM is based on a simplified conceptualization of a LNAPL release. **Figure 2** shows the geometry assumed for HSSM, which is a simplified version of the scenario described in **Figure 1**. Within HSSM, the LNAPL follows a one-dimensional path from the surface to the water table. Properties of the subsurface are taken as being uniform. The LNAPL is composed of two components: one is the LNAPL phase and the other is the chemical constituent of interest. At the water table, the LNAPL spreads radially, which implies that the regional gradient has no effect on the flow of the LNAPL. Dissolution of the chemical constituent obeys local equilibrium partitioning, but is driven by the flowing ground water and recharge water reaching the water table. The chemical constituent is transported by advection and dispersion to multiple receptor points in the uniform aquifer. Further details on these assumptions are given below.

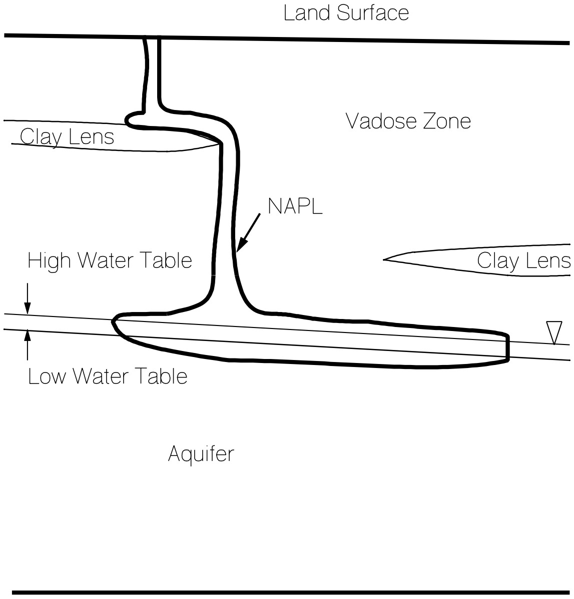


Figure 1 Schematic view of NAPL release

The model is composed of three modules, based on the simplified conceptualization presented above. All of the modules are in the form of semi-analytical solutions of the governing equations, so the modules of HSSM do not use discretization of the flow domain nor iterative solution techniques. These approximations are designed to execute rapidly. The conceptual basis of the modules are discussed in the following paragraphs. The mathematical details of the modules are found in *The Hydrocarbon Spill Screening Model (HSSM) Volume 2: Theoretical Background* (Charbeneau et al., 1994).

The model is intended to address the problem of LNAPL flow and transport from the ground surface to a water table aquifer. Assuming that the principle interest lies with water quality, an emphasis of the model is the determination of the NAPL lens size and the mass flux of contaminants into the aquifer. These quantities define the source condition for aquifer contamination and must be based upon multiphase flow phenomena in the vadose zone. The first two modules of HSSM address the vadose zone flow and transport of the LNAPL. These two are the Kinematic Oily Pollutant Transport (KOPT) and OILENS modules. KOPT and OILENS are combined into one computer code, HSSM-KO, which provides a time-variable source condition for the aquifer model.

A chemical constituent dissolved in both the LNAPL and water phases is tracked by KOPT and OILENS. Once that chemical constituent reaches the water table, it contaminates the aquifer by contact with the recharge water and by dissolution from the LNAPL lens. Thus, the third part of the model is transported through the aquifer of one chemical constituent of the LNAPL. Notably, the mass flux from OILENS is time varying, so that the aquifer model must be capable of simulating a time varying source condition. In keeping with the level of approximation used in KOPT and OILENS, one suitable choice is the Transient Source Gaussian Plume (TSGPLUME) model, which uses an analytical solution of the advection-dispersion equation. TSGPLUME uses different numerical techniques than KOPT and OILENS; so it is not incorporated within HSSM-KO, but rather is implemented in the computer code HSSM-T. The TSGPLUME model takes the dissolution mass flux from the OILENS module of HSSM-KO and calculates the expected concentrations at a number of down gradient receptor points.

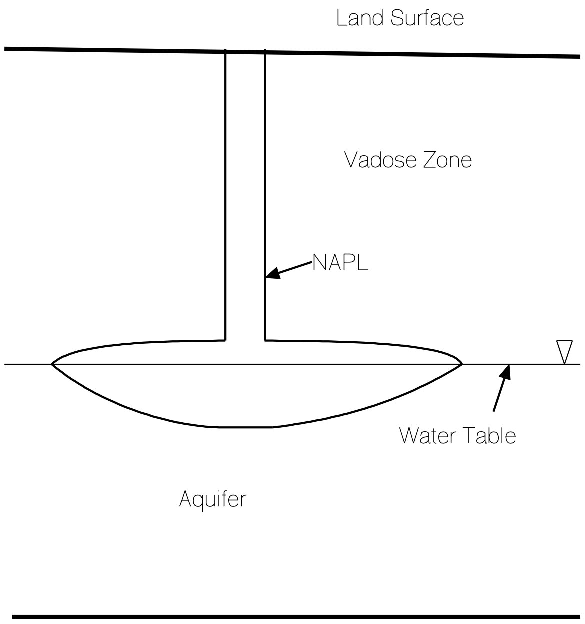


Figure 2 Schematic view of idealized NAPL release that is used in HSSM

Table 1 summarizes the component modules of the HSSM. Note that the names KOPT, OILENS and TSGPLUME refer to the mathematical models, while HSSM-KO and HSSM-T refer to the computer implementations of the models.

Table 1 Implementation of HSSM modules

Subsurface Region	Mathematical Model	Computer Code
Vadose zone	KOPT	HSSM-KO
Water table	OILENS	HSSM-KO
Aquifer	TSGPLUME	HSSM-T

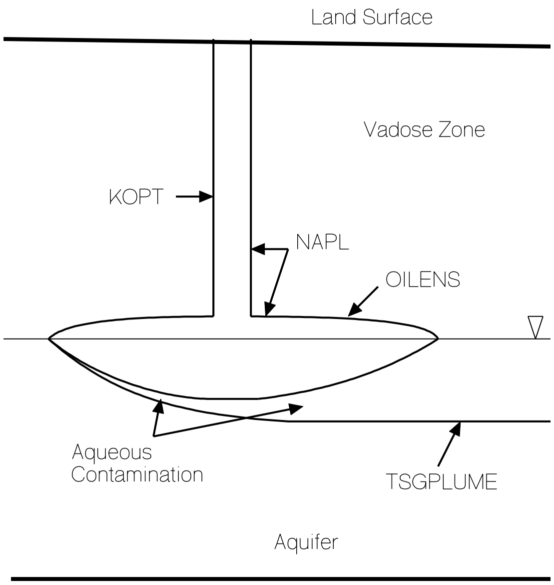


Figure 3 HSSM schematic showing the use of each module

The portion of the subsurface covered by each module of HSSM is shown in **Figure 3**. In the model scenario, the contamination is introduced as an LNAPL which flows from near the surface to the water table. This portion of the contamination event is modeled by KOPT and OILENS, as indicated on the figure. Through contact with the infiltrating recharge and the groundwater, chemical constituents of the NAPL dissolve and contaminate the aquifer. Transport of one chemical constituent of the NAPL is simulated by TSGPLUME.

1.3 Obtaining a Copy of HSSM

HSSM is available from the Center for Subsurface Modeling Support (CSMoS) at the Robert S. Kerr Environmental Research Laboratory (RSKERL). CSMoS distributes software and documentation free-of-charge through a diskette exchange program and provides technical support for the codes they distribute. To obtain the HSSM software and user documentation send a letter of request along with two high density 3.5" formatted diskettes to the following address:

Center for Subsurface Modeling Support
Robert S. Kerr Environmental Research Laboratory
United States Environmental Protection Agency
P.O. Box 1198
Ada, Oklahoma 74820
Voice: 405-436-8586
FAX: 405-436-8529

Please indicate if the DOS or Windows version is needed. If both interfaces are needed, enclose three formatted diskettes.

The complete HSSM package consists of the documents

- *The Hydrocarbon Spill Screening Model (HSSM) Volume 1: User's Guide,*
- *The Hydrocarbon Spill Screening Model (HSSM) Volume 2: Theoretical Background and Source Codes,*

and the two high density 3.5" diskettes. The diskettes contain:

For Windows:

☐ diskette HSSM-1-w The Windows Interface, HSSM-WIN

For DOS:

☐ diskette HSSM-1-d The DOS Interface, HSSM-DOS

For Windows and DOS:

☐ diskette HSSM-2 Example Problems

HSSM and the user documentation are in the public domain. They may be freely distributed or copied by anyone.

Section 2 Assumptions Underlying HSSM

The following paragraphs discuss the conceptual basis of KOPT, OILENS and TSGPLUME. This discussion is intended to give a clear understanding of the assumptions and limitations of each module of HSSM.

2.1 Kinematic Oily Pollutant Transport (KOPT)

The Kinematic Oily Pollutant Transport (KOPT) model simulates flow of the LNAPL phase and transport of a chemical constituent of the LNAPL from the surface to the water table. The LNAPL is assumed to be released at or below the ground surface in sufficient quantity to form a fluid phase that is distinct from the water. As a result, the amount of LNAPL released is far greater than that which would give only contamination dissolved in the water phase. The flow system is idealized as consisting of a circular source region overlying a water table aquifer at specified depth. Although the actual flow in the vadose zone is three-dimensional, the KOPT model treats flow and transport through the vadose zone as one-dimensional. Lateral spreading of contaminants by capillary forces is neglected, as is spreading due to heterogeneity, since the soil is assumed to be of uniform composition. For situations where the NAPL is released over a relatively large area, the actual flow is nearly one-dimensional in the center. For contaminant sources that are of small areal extent, the lateral transport of contaminants may be significant. By treating the flow as one-dimensional, however, the modeling is conservative as all of the pollutant is assumed to move downward and contribute to aquifer contamination. In actuality, some may be left behind due to entrapment by layering or lateral spreading.

The spill of the LNAPL phase may be simulated in three ways (**Figure 4**):

① The release of an LNAPL may occur at a known flux for a specified duration. This situation would occur if a known volume of LNAPL was released during a certain time period. The LNAPL volume divided by the duration and area of release determines the release rate, q_o. If the LNAPL flux exceeds the maximum effective LNAPL conductivity, K_{eo}, some of the LNAPL will run off at the surface.

② A known volume of LNAPL may be placed over a specified depth interval, d_{pl}. When the simulation begins the LNAPL may begin to flow out of the specified zone, if the LNAPL retention capacity of the soil is exceeded.

③ The last option is the specification of a constant depth of ponded LNAPL for a certain duration. This case represents a slowly leaking tank or a leaking tank within an embankment. In either of these situations, the ponded depth of NAPL is estimated or known. Two options are available for this boundary condition. In the first, the ponding abruptly goes to zero at the end of the ponding period. In the second, the ponded depth decreases gradually at the end of the ponding period.

Figure 4 HSSM release options

LNAPL phase flow is assumed to occur within the soil which contains a uniform amount of water. In KOPT, the amount of each fluid is expressed as saturation, S, which is defined as the fraction of the pore space filled by a given fluid. The water saturation corresponds to the average annual recharge rate or a specified water saturation. By using this approach, the temporal effects of climate are neglected. Justification of this approach comes from the fact that in uniform soils the soil moisture profile shows little variation except near the surface (Charbeneau and Asgian, 1991). Many data are required to simulate the time record of rainfall events to develop the non-uniform and time-variable soil moisture profile. The level of effort involved is not consistent with the intended purpose of the model as a screening methodology. Weaver (1991) presented model results which illustrate the effects of rainfalls on in-place LNAPLs. This work showed that when simulating fuels such as gasoline, the LNAPL often reaches the water table rapidly. So simulation of long sequences of rainfalls may be of little use, if the objective of the modeling is to estimate the gasoline's arrival time at the water table.

In accordance with common soil science practice (Richards, 1931), the effect of the air flow on the LNAPL phase transport is neglected in KOPT. The presence of the water and air phases is incorporated by the use of a non-hysteretic, three-phase, relative permeability model. This model is a reasonable approximation of the pore-scale phenomena occurring in three-phase flow, but the actual nature of these relationships is a major cause of uncertainty in this and most other multiphase flow models. The model uses measured properties of the soil (capillary pressure curve parameters) to approximate the relative permeability. The model does not include transport in fractures or macropores.

Figure 5 Comparison of sharp and spreading fronts

Figure 6 Comparison between experimental data and the KOPT model

Efficiency is achieved in running the model primarily by neglecting the effects of the capillary gradient on most aspects of the flow. This causes the governing equations to become hyperbolic equations, which can be solved by the generalized method of characteristics (Charbeneau et al., 1994). One major effect of this assumption on the simulation results is that the leading edge of the LNAPL moving into the soil is idealized as a sharp front (**Figure 5**). Some laboratory experiments in uniform sand packings (Reible et al.,1990) show soil NAPL profiles which have nearly sharp fronts. Similar results have been found in flow visualization experiments conducted in nearly uniform sands at the Robert S. Kerr Environmental Research Laboratory (RSKERL) and reported in Weaver et al. (1993). **Figure 6** shows an experimental result for a gasoline release into a uniform sand. Independently measured parameter values were used to simulate the experiment. It is clear that KOPT is able to simulate the main qualitative features of the flow, because the shape of the simulated NAPL front matches that of the experimental data. Quantitative agreement was obtained by adjusting parameter values within their measured ranges. The details of a similar experiment are presented in Volume 2 of the HSSM documentation (Charbeneau et al., 1994).

Since the capillary gradient has a dramatic impact on the infiltration capacity of the soil, the approximate Green-Ampt model (Green and Ampt, 1911) is used to estimate the infiltration capacity during the application of the LNAPL phase. This gives an improved estimate of flux in the soil, given a flux or constant head ponding condition at the surface.

In KOPT and OILENS, the LNAPL is treated as a two-component mixture. The LNAPL itself is assumed to be soluble in water and sorbing. Due to the effects of the recharge water and contact with the ground water, the LNAPL may be dissolved. This may be significant for highly soluble LNAPL phases. The LNAPL's transport properties (density, viscosity, capillary pressure, relative permeability), however, are assumed to be unchanging. The second component is the chemical constituent which can partition between the LNAPL phase, water phase and the soil. This constituent of the LNAPL is considered the primary contaminant of interest. Concentrations of this constituent are reported in the model output and graphed by the post-processors.

A kinematic approach is used by KOPT for transport of the chemical constituent, which results in a model that neglects dispersion. The chemical motion is assumed to be caused by the advection of water and LNAPL only. Hydrophobic contaminants that reside primarily in the LNAPL phase will largely be transport with the LNAPL. The chemical constituent, which is the second component of the LNAPL phase discussed above, is assumed to partition between the NAPL, water and soil according to equilibrium, linear partitioning relationships. The constituent mass flux into the aquifer comes from recharge water that is contaminated by contact with the lens and from dissolution that occurs as ground water flows under the lens. The concentration of the chemical in the aquifer is limited by its effective mixture solubility, which is less than its pure phase solubility in water.

2.2 OILENS

If a large enough volume of hydrocarbon is released, then the LNAPL reaches the water table. Typically this occurs in a relatively short time for LNAPLs, like gasoline, that have low viscosities. The OILENS module simulates radial spreading of the LNAPL phase at the water table and dissolution of the chemical constituent. If sufficient head is available, the water table is displaced downward; lateral spreading begins; and the OILENS portion of the model is triggered. OILENS is based on three major approximations. First, the LNAPL spreading is purely radial, which implies that the slope of the regional ground water table is small enough to be unimportant for the lens motion. Second, the thickness is determined by buoyancy alone (Ghyben-Herzberg relations). Third, the shape of the lens is given by the Dupuit assumptions, where flow is assumed horizontal and the gradient is approximated by the change in head over a horizontal distance. These three assumptions lead to an efficient formulation of the model, which is reflected in its low computational requirements.

The lens thickness in the formation and the lens radius both increase during the initial phase of spreading (**Figure 2**). The height of the lens depends on the LNAPL phase density and viscosity, the release characteristics, and the saturated hydraulic conductivity of the system. For example, in a given porous medium, diesel fuel would tend to form taller lenses than gasoline because of its higher viscosity. Initially the lenses build up height because the LNAPL enters the lens at a higher rate than it moves radially. Later, after the source rate declines, the lens thins while continuing to spread laterally. Residual hydrocarbon is left both above and below the actively spreading lens during this period (**Figure 7**). The thickness calculated by OILENS is an averaged thickness of the LNAPL in the formation (Appendix 3.3, Schwille, 1967) and is not necessarily directly related to the thicknesses observed in observation wells (Kemblowski and Chiang, 1990).

Figure 7 Lens configuration during thinning phase

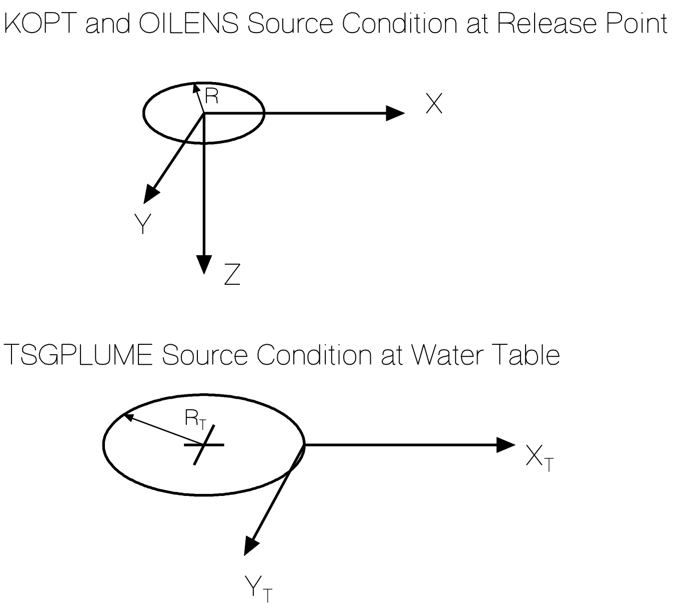
Figure 8 Gaussian source configuration used in TSGPLUME

2.3 Transient Source Gaussian Plume Model (TSGPLUME)

Aquifer transport of the chemical constituent is simulated by the Transient Source Gaussian Plume Model (TSGPLUME) which uses a two-dimensional vertically averaged analytical solution of the advection-dispersion equation. Two important considerations are the boundary condition for the aquifer and the assumptions used in applying the two-dimensional planar model.

The boundary conditions are placed at the down gradient edge of the lens and take the form of a Gaussian concentration distribution with the peak directly down gradient of the center of the lens (**Figure 8**). The peak concentration of the Gaussian distribution adjusts through time so that the simulated mass flux from the lens equals that going into the aquifer. The width of the Gaussian distribution remains constant and is taken so that four standard deviations are equal to a representative diameter of the lens. Although the size of the lens varies with time, a constant diameter is used in TSGPLUME for the aquifer source condition. A reasonable choice for the lens diameter is the diameter that occurs when the mass flux into the aquifer is a maximum. This choice assures that the peak mass flux into the aquifer occurs through an appropriately-sized lens.

Although the aquifer model is two-dimensional in the horizontal plane, complete mixing of the chemical over the aquifer thickness is neither necessary nor assumed a priori. Vertical mixing is represented by the depth of penetration of the plume into the aquifer and is calculated from the amount of vertical dispersion beneath the lens plus the advective flow due to infiltration through the lens, following the approach of Huyakorn et al. (1982). If the calculated penetration depth exceeds the aquifer thickness, then the plume fully penetrates the aquifer; and the model allows for dilution of the plume by diffuse recharge. If the penetration depth is less than the aquifer thickness, then the plume thickness is taken as the penetration depth. In the latter case, recharge simply pushes the plume deeper and the penetration thickness remains constant.



KOPT and OILENS Source Condition at Release Point

TSGPLUME Source Condition at Water Table

Figure 9 Coordinate systems for the KOPT, OILENS and TSGPLUME Modules of HSSM

Figure 9 shows the coordinate systems for all three modules of the HSSM model. For KOPT and OILENS, the source of contamination is assumed to be a circle of radius, R_s, located at the ground surface. The coordinate origin is located at the center of the source. X is the down gradient direction, and Y is the transverse horizontal direction. The Z axis points downward, so that the depth is equal to the Z coordinate value. In TSGPLUME, the source of contamination is assumed to be a circle of radius R_T, located at the water table. The size of the source is taken as a radius calculated in the OILENS module. The coordinate origin (X_T,Y_T) is assumed to be at the down gradient edge of the source of contamination. The HSSM-T implementation of TSGPLUME adjusts the X coordinates used by HSSM-KO to the X_T values needed by TSGPLUME ($X_T = X - R_T$). The coordinates written in the output and plot files are the coordinates used by KOPT and OILENS (X,Y,Z).

In TSGPLUME, the water flow is assumed to be one-dimensional, so advection of the contaminant is simulated only in the longitudinal (X_T) ground direction. The constituent may be transported by dispersion, however, both longitudinally (X_T) and transversely (Y_T). As with many analytical solutions, the aquifer is assumed uniform. The mass flux into the aquifer varies with time, and the concentration history at the receptor point is determined by integration of the constant input solution and the variable mass flux distribution into the aquifer.

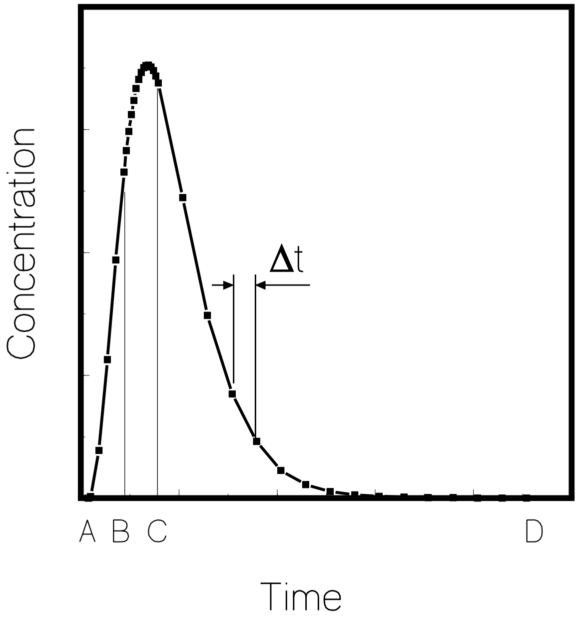


Figure 10 Schematic representation of a TSGPLUME concentration history

The results from TSGPLUME are concentration histories at user-specified receptor points. At these points, the model calculates the aqueous phase concentration of the contaminant beginning at the time at which the concentration first rises above a threshold value (time A on **Figure 10**). This time is determined by a search algorithm which uses the analytical solution to determine the earliest time at which the concentration is above the threshold. Typically the threshold value is set to 1 ppb by the model user. Calculation of the receptor concentration continues at intervals of Δt, as set by the user. The time interval is shortened at time B to a small value in order to capture the peak concentration. If necessary, the step is further shortened in order to make sure that the peak is found. Once the concentration is reduced below the peak (time C), the time step increases gradually to again equal the original Δt. Calculation continues until the concentration drops below the threshold (time D).

Section 3 HSSM Interface Options

Two interfaces are provided to assist the user in running the HSSM. The first interface was developed for the Microsoft Windows operating system. This interface consists of the windows interface program, HSSM-WIN, and the two simulation programs: HSSM-KO and HSSM-T. HSSM-WIN is used to create and edit input data sets, execute HSSM-KO and HSSM-T, and plot the model results. The windows interface is described in Section 4, titled "The MS-Windows Interface, HSSM-WIN."

Table 2 Comparison of MS-DOS and MS-Windows Interfaces

Interface	Advantages	Disadvantages
DOS	1. The fastest performance of model calculations is achieved (for any given computer) under the DOS interface. 2. DOS interface can run on a machine with limited processing power and limited RAM. The code will execute, albeit slowly, on a 286 machine with 640 kiloBytes of RAM.	1. The DOS preprocessor is interactive but not graphical.
Windows	1. A single shell program performs all necessary functions of the model.	1. The calculations performed by HSSM-KO and HSSM-T are slower under the Windows interface due to Windows overhead.
	2. Data are entered directly on graphical screens.	2. Requires a machine with enough processing power and memory to run Windows effectively. Typically this would be a 386 or higher with at least 4 megaBytes of RAM.
	3. Simultaneous display of all model output.	3. Requires a certain level of expertise with Windows.
	4. Simultaneous display of output from simulations with different parameter values.	4. More system memory is consumed by Windows than by DOS.
	5. Ability to cut and paste to other Windows applications.	

The second interface was developed for the MS-DOS operating system. In this case the interface consists of four programs: PRE-HSSM, HSSM-KO, HSSM-T, and HSSM-PLT. PRE-HSSM is used to create and edit input data files; HSSM-KO and HSSM-T perform the model calculations, and HSSM-PLT is used to plot and output the model results. The four programs can be run individually or the HSSM-DOS program can be used as a simple menu system. The DOS interface is described in Appendix 1 "The MS-DOS Interface, HSSM-DOS."

Each of the interfaces can be used to create and edit input data files, run the model, and plot the results. The Microsoft Windows interface allows extensive manipulation of the model output, concurrent display of all of the main outputs of the model, and concurrent display of results from several simulations. To aid in selecting a user interface, Table 2 describes some advantages and disadvantages of each interface. Detailed information on running the HSSM under each of the interfaces is given in the respective section or appendix. Each contains the same information on estimation of the model parameter values, so that the user has the parameter information available where its input procedures are described.

Three utility programs are provided to simplify calculation of values of certain input parameters. The utilities, which are listed in Table 3, are referenced as necessary where the parameter values are described. Background information and instructions for running the utilities are provided in appendices.

Table 3 HSSM Data Calculation Utilities

Parameter(s)	Utility Program Name
Soil Hydraulic Properties	SOPROP
Equilibrium NAPL/water partition coefficients	RAOULT
Average NAPL saturation for OILENS	NTHICK

3.1 Typographical Conventions

The typographical conventions shown in Table 4 are used throughout the user's guide.

Table 4 Typographical Conventions

Type style	Use
PROGRAM	Program names are written in capitals. For example: HSSM-WIN, HSSM-DOS, HSSM-KO, and HSSM-T.
new term	Italic type usually signals a new term.
KEYBOARD	Small capitals are used to identify the names of keys on the keyboard like CTRL, F1, or ESC.
FILE.DAT	Filenames appear in this typeface. Specific references to the program files also use this typeface, for example: **HSSM-KO.EXE** refers to the file which contains the HSSM-KO program.
`COMMAND`	Commands entered at the DOS prompt and ASCII messages written to the screen by DOS programs.

Section 4 The MS-Windows Interface, HSSM-WIN

The MS-Windows interface, HSSM-WIN, provides a convenient interface for creating and editing data files, running HSSM, visualizing the output from several runs at one time, and exporting graphics into other Windows applications. This interface was developed from the ShowFlow Modeling Interface developed at the University of Texas at Austin (Tauxe, 1990) and is described in this section of the user's guide.

4.1 Microsoft Windows Interface Overview

The main functions of the interface are outlined in Table 5. Necessary details are provided in the sections noted in the table.

Table 5 Outline of the HSSM-WIN Interface

Interface Function	Section References
1. Installation of HSSM-WIN	4.2 and 4.3
2. Operation of the HSSM-WIN Interface, Summary of Interface Commands	4.4
3. Creation of Data Sets	4.5
4. Editing of Input Parameters	4.6.1 and 4.6.3 to 4.6.6
5. Running HSSM-KO and HSSM-T	4.5.3, 4.7
6. Graphing HSSM Results	4.5.4
7. Interpretation of HSSM Graphs	4.8
8. HSSM Output File Contents	6

The general procedure for using HSSM-WIN follows. After installing HSSM-WIN, a data set must be created by selecting the HSSM-WIN "Edit" menu item (Section 4.5). HSSM-WIN contains four data editing screens (called dialog boxes) that are used in succession to create the complete input data sets for HSSM-KO and HSSM-T (Sections 4.6.1 and 4.6.3 to 4.6.6). Once the user is satisfied with the data set, then the data are saved to a new file name or an existing file may be overwritten. This file name is loaded into HSSM-WIN's memory and will be used when the simulation is performed.

HSSM-KO and HSSM-T are executed from the Windows interface. Since HSSM-KO and HSSM-T are independent programs, they must be run in succession to complete the entire simulation. Section 4.7 describes the execution of these programs. Once each has finished, a DOS window remains on screen that the user must close before proceeding. This feature is provided because it is important to see the screen messages that are written by the programs. (Windows would normally close the DOS window immediately upon completion of the programs and the user would not be able to see the final set of messages.)

When a simulation is completed, the results may be graphed with the HSSM-WIN Graph menu item. Six graphs can be displayed by the interface, and the user may select those he/she would like to view (Section 4.5.4). HSSM-WIN allows copying of graphs to other Windows applications (Section 4.5.8), simultaneous display of results from multiple simulations (Section 4.5.7), and printing of the graphs (Section 4.5.6).

4.2 System Requirements

HSSM-WIN is an application written for the Microsoft Windows graphical environment. To use the Windows interface the user should be generally familiar with personal computers, DOS, Windows, and the HSSM model. Users are advised to learn various features of Windows, as many of the capabilities of HSSM-WIN require knowledge of Windows functions. There are several requirements for your system:

HARDWARE:

- For *386 enhanced mode*, a personal computer with the Intel 80386 processor (or higher) and 2 megabytes (MB) or more of memory (640K conventional memory and at least 1024K of extended memory).

  For *standard mode*, a personal computer with the Intel 80286 processor (or higher) and 1 megabyte or more of memory (640K conventional memory and at least 256K extended memory).

  For *real mode*, a personal computer with the Intel 8086 or 8088 processor (or higher) and 640K conventional memory. Windows 3.1 and later do not support real mode.

- A hard disk and at least one floppy disk drive.

- A video monitor supported by Windows (EGA or better resolution).

- A printer supported by Windows.

- A mouse that is supported by Windows is strongly recommended.

The amount of system memory available under Windows may be checked by opening a DOS window and typing the DOS `MEM` command. The amount of memory available for running a DOS application will be displayed. This amount must exceed the approximately 400 kbytes required by HSSM-KO. If sufficient memory is not available under Windows, HSSM-KO and HSSM-T may be run under DOS and the results later plotted by HSSM-WIN.

SOFTWARE:

- Microsoft Windows version 3.0 or later.

- Windows requires MS-DOS or PC-DOS version 3.1 or later.

4.3 Installation

4.3.1 Packing List of Files

Table 6 shows the files that are found on the HSSM-WIN distribution diskette, HSSM-1-w.

Table 6 Packing list of files for the HSSM Windows interface

File	Purpose
HSSM-WIN.EXE	The Windows interface program
HSSM-KO.EXE	The KOPT and OILENS modules of HSSM
HSSM-T.EXE	The TSGPLUME module of HSSM
HSSM-KO.PIF	A Windows program information file (pif) for **HSSM-KO.EXE**
HSSM-T.PIF	A Windows program information file (pif) for **HSSM-T.EXE**
REBUILD.EXE	A recovery program for interrupted simulations
REBUILD.PIF	A Windows program information file (pif) for **REBUILD.EXE**
HSSMHELP.WRI	The HSSM-WIN help file, which can be read by Windows WRITE (the word processor bundled with Windows).
README.TXT	This file contains information on changes which have occurred since the writing of the user's guide.
RAOULT.EXE	Utility to perform Raoult's Law Calculation
RAOULT.DAT	Default data set for the RAOULT utility
SOPROP.EXE	Utility to estimate soil properties with Rawls and Brakensiek's (1985) regression equations.
NTHICK.EXE	Utility to estimate NAPL thickness at the water table
SYSTEM\COMMDLG.DLL	Windows dynamic link library provided for users of Windows 3.0

Several example problems, including those presented in Section 5, are distributed on diskette HSSM-2. Be sure to back up these files on other diskettes and to write-protect the distribution diskettes.

4.3.2 Copying Files to the Hard Drive

This section describes the installation of HSSM-WIN from DOS, which is the simplest installation procedure. Check the **README.TXT** file for information on automated installation procedures which are under development as of this writing. Experienced users of Windows can install the program using Window's File Manager. For further information on File Manager, consult your Windows reference materials.

After backing up the HSSM-1-w diskette, create a sub-directory for the model by entering the DOS command:

```
MKDIR C:\HSSM
```

where HSSM is the name of the HSSM-WIN subdirectory. With the HSSM-1-w diskette in drive A, copy all of the files from the diskette to the HSSM directory on the hard drive by entering:

```
COPY A:\*.* C:\HSSM
```

(The HSSM-1-w diskette may be in another drive, say B, by entering `"B:"` rather than `"A:"` in the previous command.) The example problems and output files contained on diskette HSSM-2 should be installed into a separate directory. Create the example problem directory by entering:

```
MKDIR C:\HSSM\EXAMPLE
```

The files are copied to this directory by entering:

```
COPY A:\*.* C:\HSSM\EXAMPLE
```

Subdirectories can and should be created for each HSSM simulation. For example, to create a directory PROJECT1, enter the command:

```
MKDIR C:\HSSM\PROJECT1
```

By selecting the `PROJECT1` subdirectory when using HSSM, all the input and output files for the simulation will be in `C:\HSSM\PROJECT1`.

Users of Windows 3.0 will also need to copy the dynamic link library COMMDLG.DLL from the SYSTEM subdirectory on the distribution diskette to the SYSTEM subdirectory of their windows directory on the hard disk by entering:

```
COPY A:\SYSTEM\COMMDLG.DLL C:\WINDOWS\SYSTEM
```

Windows 3.1 users already have this file. The user will now likely wish to add HSSM-WIN to a program manager group as described in the next section.

4.3.3 Adding HSSM to a Program Manager Group

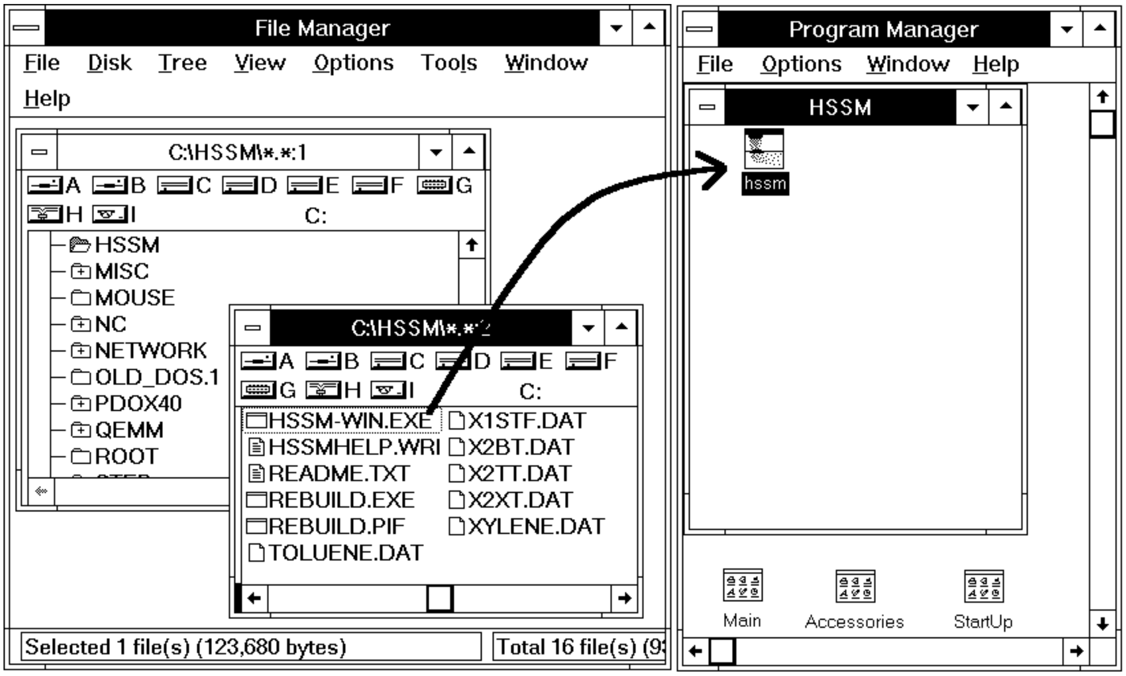
The HSSM-WIN program should be added to a Program Manager group so that HSSM-WIN can be executed by clicking on its icon. Two procedures are given for this operation:

① With both the File Manager and Program Manager occupying different places on the screen as in **Figure 11**, simply drag the file name **HSSM-WIN.EXE** to the desired Program Manager group, where it will appear as an icon.

② Alternatively, you may use the "File" "New" command of Windows to specify a new program group and item.

<u>For the program group:</u>
Select the Program Group radio button
Click on the "OK" button
Enter `HSSM` as the Description
Click on the "OK" button

<u>For the program item:</u>
Select the Program Item radio button
Click on the "OK" button
Enter `HSSM` as the Description
Enter `C:\HSSM\HSSM-WIN.EXE` as the Command line
Enter `C:\HSSM` as the Working Directory
Click on the "OK" button



Selected 1 file(s) (123,680 bytes)

Total 16 file(s) (9

Figure 11 Installing HSSM-WIN in a Program Manager group

Once HSSM-WIN has been successfully loaded onto your system, you must check the **CONFIG.SYS** file. The HSSM-KO program opens a number of temporary files and **CONFIG.SYS** must be configured so that a sufficient number of files may be opened. The **CONFIG.SYS** on your system needs to include the line

```
FILES = 30
```

(A number greater than thirty will also work.) After modifying **CONFIG.SYS** you must reboot your system to allow the change to take effect. Installation of both the Windows and DOS interfaces on one computer is discussed in Appendix 9.

4.4 Using HSSM-WIN

4.4.1 Starting Up

Like other Windows applications, HSSM-WIN will appear in a Program Manager group as an icon, and can be started simply by double clicking with the mouse cursor on the icon.

HSSM-WIN can also be started from Windows' File Manager by double-clicking on the file named **HSSM-WIN.EXE** with the mouse pointer. If you do not have a mouse, choose "Run..." from the "File" menu (ALT+F followed by R) and enter "C:\HSSM\HSSM-WIN.EXE" in the prompt box. The screen will clear and the main window of HSSM-WIN will appear.

A variety of menu options appears in the *menu bar* along the top of the HSSM-WIN window (**Figure 12**). These menu options are headings for related operations which will appear in a *pull-down menu* below each menu item. For more information on using the standard Windows interface consult your Windows documentation.

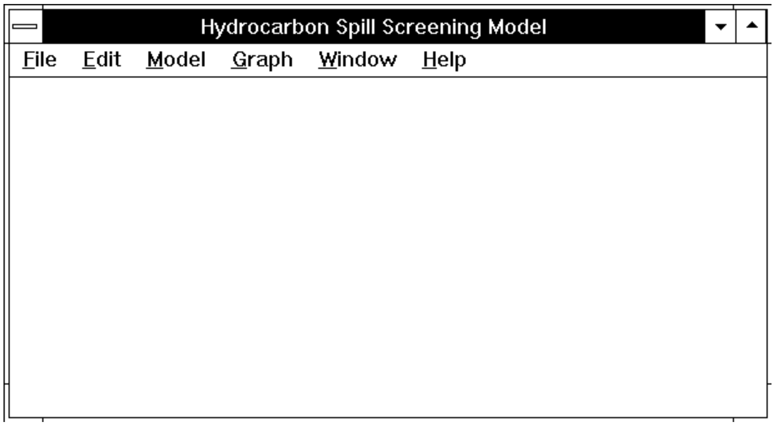


Figure 12 The initial HSSM-WIN screen

When HSSM-WIN first appears on the screen, some menu items are written in a different color, or *disabled*. This means that those commands are not available at this time, since no data nor parameters have yet been loaded into the program. For example, the Save and Graph commands are disabled since no data yet exist to save or graph. The available options include File Open and Edit, to open an existing input file or edit one from scratch. Once data have been loaded, all of the menu options become available.

4.4.2 Menu Command Summary

Table 7 contains a listing of all HSSM-WIN commands. Every HSSM-WIN command is either

① a menu option of the main menu bar (column headings 1 to 6 of Table 7, see **Figure 12**),
② listed in a pull-down menu (entries in columns 1 to 6 of Table 7), or
③ listed in the system menu (entries in column 7 of Table 7).

(The system menu is accessed by clicking on the icon in the upper left corner of the window or by pressing ALT + SPACEBAR on the keyboard). Some of the commands are followed by an ellipsis (...), which means that more information is requested before executing. A menu item in HSSM-WIN may have one letter underlined, or it may be followed by an *accelerator* (such as "Graph Results Ctrl+G"). These are shortcut codes for the keyboard. The user who is familiar with the program may find that the keyboard is often faster than the mouse. A description of each command is presented in Section 4.10

Table 7 HSSM-WIN Command Summary

	File (1)	Edit (2)	Model (3)	Graph (4)	Window (5)	Help (6)	System Menu (7)
(a)	New	General Data...	Run HSSM-KO	Graph Results...	Cascade	Read Help File	Restore
(b)	Open...	Hydrologic Data...	Run HSSM-T	Copy Graph	Tile	About HSSM...	Size
(c)	Save	Hydrocarbon Phase Data...	Run REBUILD	Print Graph	Arrange Icons	About HSSM-WIN..	Move
(d)	Save as ...	Model Simulation Data...		Close Graph	Close All		Minimize
(e)	✓ Check File times			Fonts	(list of graphs)		Maximize
(f)	Exit HSSM-WIN						Close
(g)							Switch to...

4.5 Use of HSSM-WIN Commands for Performing HSSM Simulations

The following sections give the specific procedures for running HSSM Simulations using HSSM-WIN commands. HSSM-WIN menu options are referred to by the column number and row letter in Table 7. For example, the Open option of menu bar item File is designated *1.b*.

4.5.1 Creating New Input Data Sets

① Clear any existing data and file names by selecting "New" from the "File" menu *(1.a)*. This step can be skipped if no files have been used previously in the current HSSM-WIN session.

② Call the Input File Editor by choosing "Edit" *(2)* from the HSSM-WIN menu (or use the accelerator Ctrl+E).

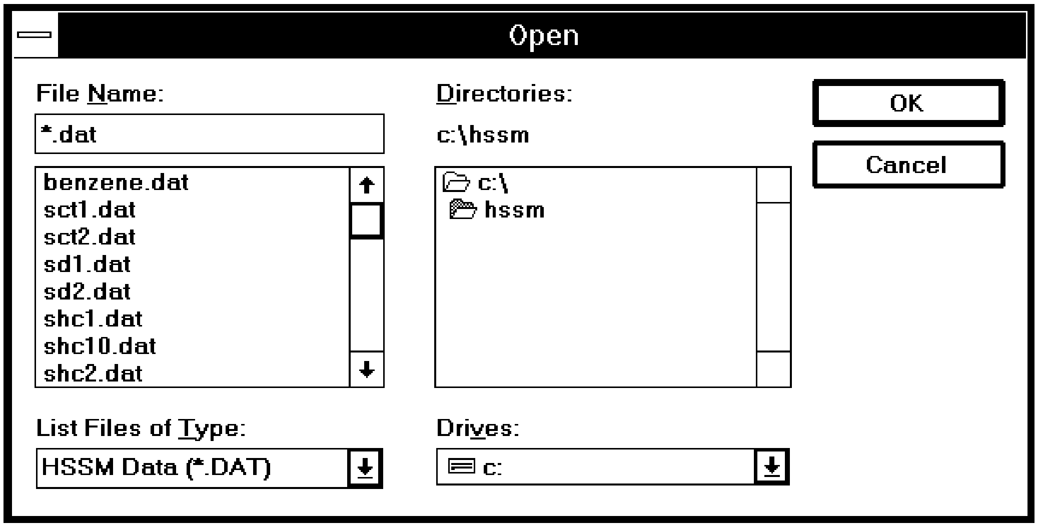
③ Enter data in each of the four Input File Editors *(2.a* through *2.d)* as described in the Sections 4.6.3 to 4.6.6, and click on "OK" (ENTER) to exit the editor.

④ Save the file with the "Save" command from the "File" menu (*1.c).* When asked for a new file name, enter a name of up to eight characters. There is no need to add the **.DAT** extension, as HSSM-WIN will do this.

4.5.2 Editing Existing Input Data Sets

① Open an existing input file for editing by following the procedure given below:

Choose the "Open..." option from the "File" menu *(1.b)*. The Open Files dialog box will list the relevant file names in the default directory, as shown in **Figure 13**.



File Name: *.dat

benzene.dat
sct1.dat
sct2.dat
sd1.dat
sd2.dat
shc1.dat
shc10.dat
shc2.dat

Directories: c:\hssm

c:\
hssm

List Files of Type: HSSM Data (*.DAT)

Drives: c:

Figure 13 File Open dialog box

Scroll through the list of names using the scroll bar with the mouse.

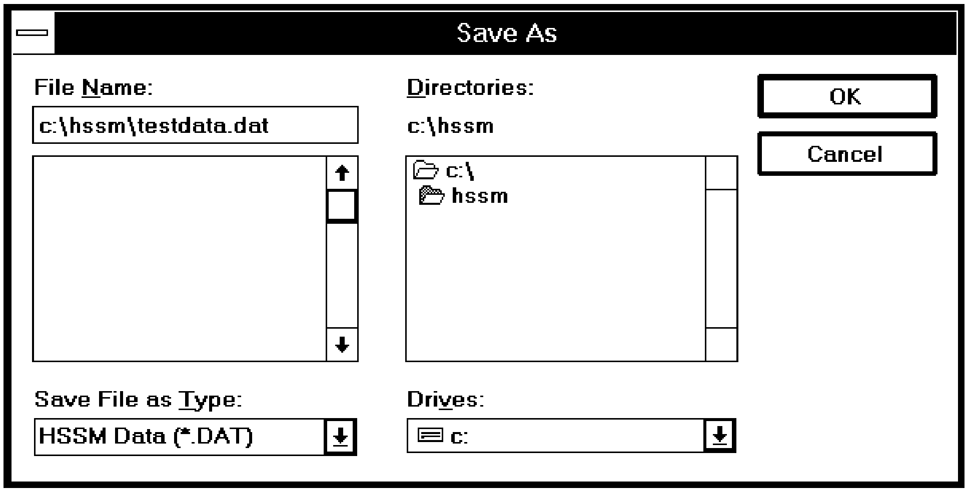
If the name of the desired file is listed here, double-click on the name to open it. (With the keyboard, type the name in the box and choose ENTER to open the file. If you decide not to open a file, choose ESC to cancel.)

② Call the Input File Editor by choosing "Edit" *(2)* from the HSSM-WIN menu (or use the accelerator Ctrl+E).

③ Enter data in each of the four Input File Editors *(2.a* through *2.d)* as described in the Sections 4.6.3 to 4.6.6, and click on "OK" (ENTER) to exit the editor.

④ Save the file.

- If you want to overwrite the original file, simply choose the "Save" option from the "File" menu *(1.c)*.
- If you want to select a new name with the "SaveAs" command from the HSSM-WIN "File" menu *(1.d)*. When asked for a new file name, enter a name of up to eight characters. There is no need to add the **.DAT** extension, as HSSM-WIN will do this.



File Name: c:\hssm\testdata.dat

Directories: c:\hssm

Save File as Type: HSSM Data (*.DAT)

Drives: c:

Figure 14 File Save As dialog box

4.5.3 Running the Model

Choose "Model" *(3)* to perform the two parts of the HSSM calculations.

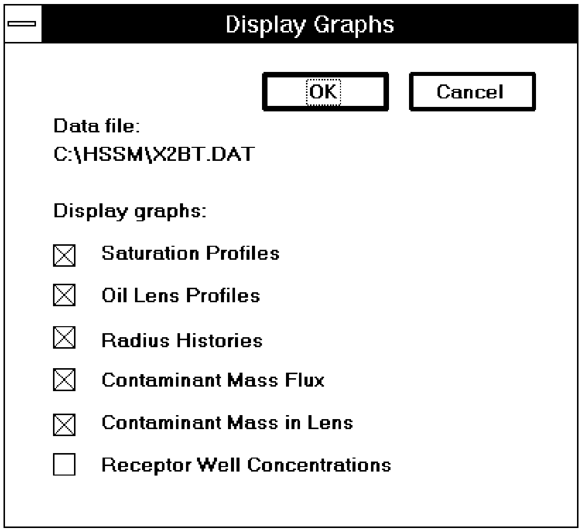
① HSSM-KO is executed by selecting "Run HSSM-KO " *(3.a)*. HSSM-KO reads the entire input data file and performs the KOPT and OILENS simulations. HSSM-KO then produces a separate input data file for HSSM-T, which contains some of the HSSM-KO input data and some of the HSSM-KO results that are needed by HSSM-T.

② After the successful completion of HSSM-KO, the second step is to run HSSM-T, by selecting "Run HSSM-T" *(3.b)*. These two programs are DOS programs, so Windows must create DOS processes in order to run these codes. Section 4.7 shows the screen messages produced when HSSM-KO and HSSM-T are executed.

NOTE: If the parameters for TSGPLUME (HSSM-T) need to be changed after HSSM-KO has been executed, the data set must be edited and HSSM-KO must be run again.

4.5.4 Graphing the Model Results

① To generate graphs of the data, choose "Graph" *(4)* and "Graph Results..." *(4.a)* to get the Display Graphs dialog box (**Figure 15**).



Data file:
C:\HSSM\X2BT.DAT

Display graphs:

☒ Saturation Profiles
☒ Oil Lens Profiles
☒ Radius Histories
☒ Contaminant Mass Flux
☒ Contaminant Mass in Lens
☐ Receptor Well Concentrations

Figure 15 Display Graphs dialog box

② Choose which graphs to make by clicking on the check boxes. An "X" in the box means that it has been selected. To do this from the keyboard, press the TAB key to move the highlight to the desired checkbox and SPACEBAR to turn the check on or off.

③ Choose "OK" to draw the graphs.

④ To close a graph, choose "Close" from the graph window's system menu, or *(4.d)* double-click with the mouse on the system menu icon in the upper left corner of the graph window. Closing unneeded graphs makes more room in memory for other graphs or programs.

4.5.5 Graphing Results From a Previous Simulation

① Load the data set by selecting "Open" from the "File" menu *(1.b)*.

② To generate graphs of the data, choose "Graph" *(4)* and "Graph Results..." *(4.a)* to get the graph dialog box.

③ Choose which graphs to make by clicking on the check boxes. An "X" in the box means that it has been selected. To do this from the keyboard, press the TAB key to move the highlight to the desired checkbox and SPACEBAR to turn the check on or off.

④ Choose "OK" to draw the graphs.

⑤ To close a graph, choose "Close" from the graph window's system menu, or *(4.d)* double-click with the mouse on the system menu icon in the upper left corner of the graph window. Closing unneeded graphs makes more room in memory for other graphs or programs.

4.5.6 Printing a Graph

① Generate a graph as described above.

② From the "Graph" menu, choose the "Print Graph" *(4.c)* option.

③ After a few seconds, a message reading "Sending graph to print manager" will appear, with the option to cancel the print job. Unless the job is to be canceled, wait until the message disappears. This means that the image has been sent on its way, and HSSM-WIN is ready to continue.

NOTE: Small graphs will print relatively quickly, but larger images will take longer. A full-page graph may take several minutes, depending on the sophistication of the printer and printer driver software and on availability of free memory and hard disk space.

4.5.7 Comparing Several Simulations

① Edit or create an input file, run the simulation, and graph the results. If the simulations have already been run and the plot files exist, then load the file name with "Open" and "File" *(1.b)*, and choose the "Graph" command to display the graphs *(4.a)*. Using the Minimize command, reduce each of the graphs to an icon. The icons will be displayed along the bottom of the HSSM-WIN window. Do this for the simulations you wish to compare.

② Restore the graphs which you wish to compare by either double-clicking on the icon or selecting from the graphs listed in the "Window" pull-down menu *(5.e)*. You may choose as many graphs as you wish.

③ Use the "Tile" command under the "Window" menu *(5.b)* to redraw the graphs as in **Figure 16**.

④ If you desire, the graph windows may be resized to match scales by "dragging" the corners or sides with the mouse or by using the Move and Size commands from the graph window's system menu *(7.c* and *7.d)*.

⑤ To view the parameter values for a particular run, open the file in question and view the data using the Input File Editors *(2.a* through *2.d)*.

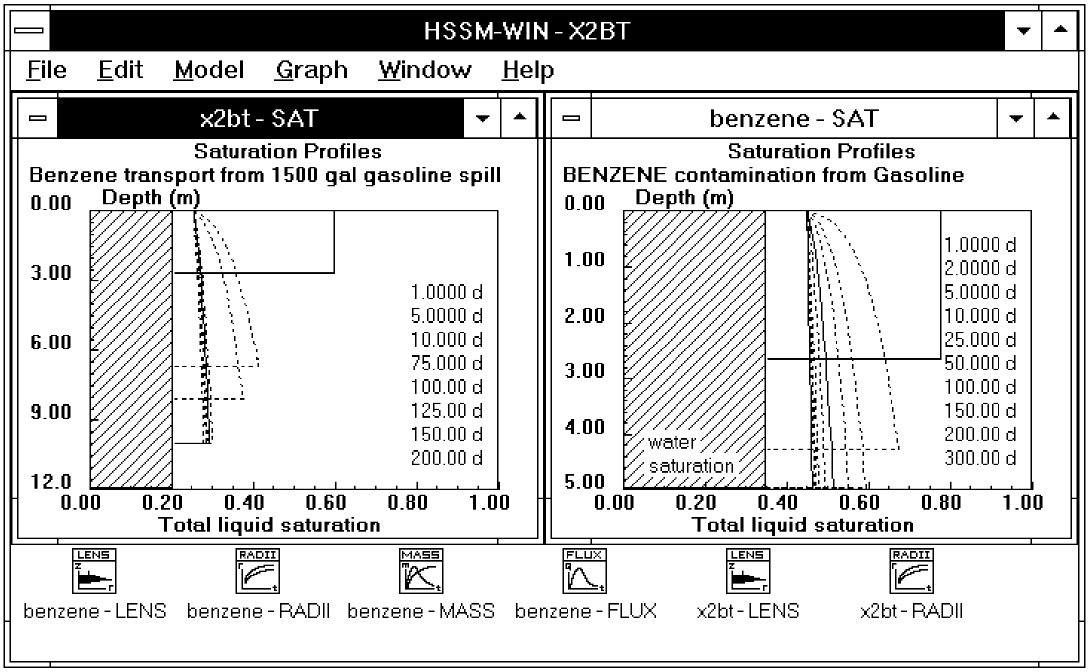


Figure 16 Comparison of Graphs from Two Different Simulations

NOTE: Each graph on the screen consumes up to a few KB of memory which are freed on closing the graph window. With several graphs and/or other applications running, HSSM-WIN or Windows may determine that there is not enough free memory or resources to create another graph. In this case, the user will be asked to terminate something to create more room in memory.

4.5.8 Copying a Graph to the Clipboard

Windows programs have the ability to transfer screen images directly from one Windows application to another. For example, an HSSM-WIN graph can be copied into a word processor document. The Windows Clipboard is used as an intermediate storage point for such transfers.

① Generate a graph as described above.

② From the "Graph" menu *(4)*, choose the "Copy Graph" option *(4.b)*. This copies the graph to the Clipboard in a bitmapped format and replaces any previous Clipboard data.

③ To see the contents of the Clipboard at any time, run the Clipboard program.

④ To paste the graph into another application, find the "Paste" command in that application's menu, if available. It should be listed under the "Edit" pull-down menu. **Figure 17** shows an HSSM-WIN graph pasted into PAINTBRUSH.

⑤ Bitmaps copied to the Clipboard can be saved as ***.CLP** files as well, so that graphs may be kept for later use.

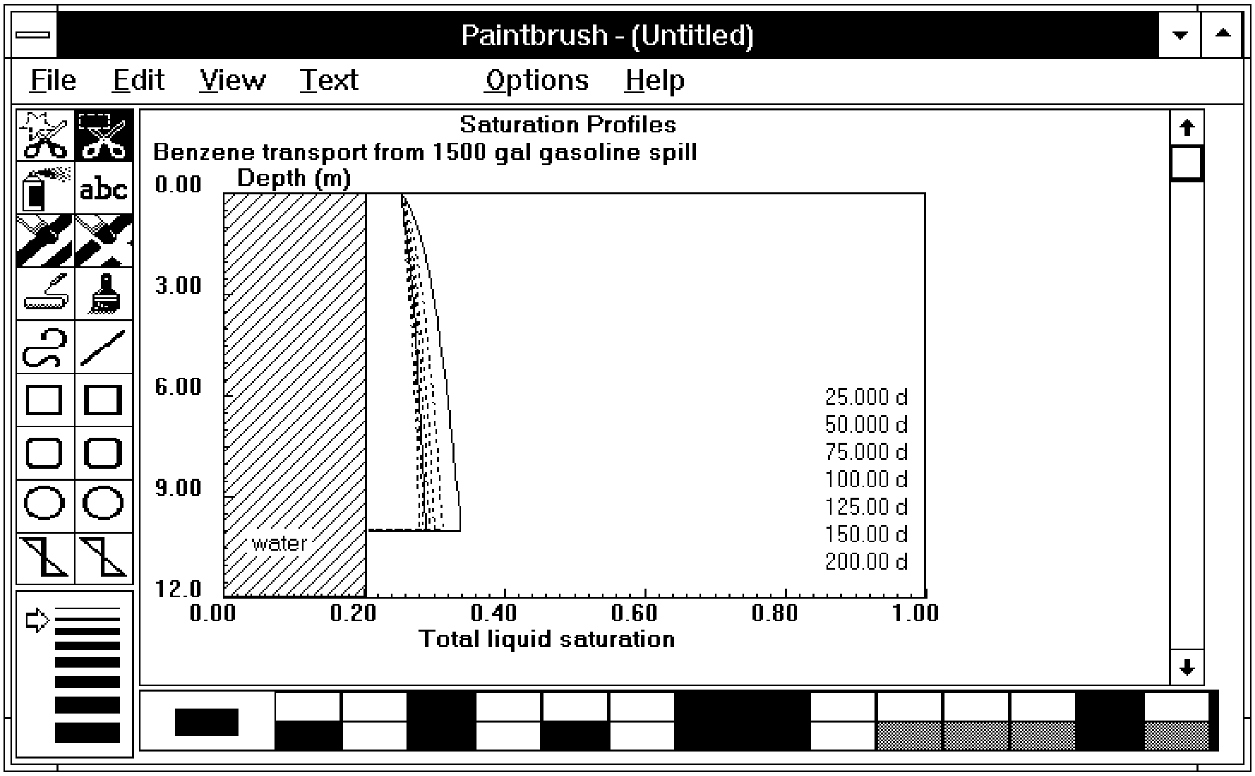


Figure 17 HSSM-WIN graph pasted into PAINTBRUSH

4.5.9 Exiting HSSM-WIN

HSSM-Win can be exited by selecting the "File" and "Exit HSSM-WIN" *(1.f)*. The program may also be exited by double-clicking on the system menu in the upper left corner (equivalent to selecting *7.f*). If any work has not been saved, HSSM-WIN will alert the user to save it before the program closes down.

4.6 Editing and Creating HSSM Data Sets

The following sections describe all the required parameters for HSSM. The sections also provide guidance on how to determine appropriate values of the parameters. For convenience, blank templates of each of these screens are provided in Appendix 13. These templates are useful for assembling data sets and may be copied for repeated use. Experienced users of the model may wish to edit their data sets directly; Appendix 10 shows the structure of the HSSM-KO and HSSM-T input data files.

4.6.1 Using the Input File Editors - Common Techniques

The following are instructions for using the Editor for the input data screens (called dialog boxes). Each of the dialog boxes requires the usage of the features described below.

① The Input File Editor dialog boxes are HSSM-WIN's method of editing the input file for the models. They are displayed by choosing the "Edit" and one of the data options from HSSM-WIN's menu. This section discusses general techniques for navigating around and editing data in these dialog boxes, that are illustrated in **Figure 19** to **Figure 22**.

② Standard Windows methods for selecting and editing text are adopted by HSSM-WIN:

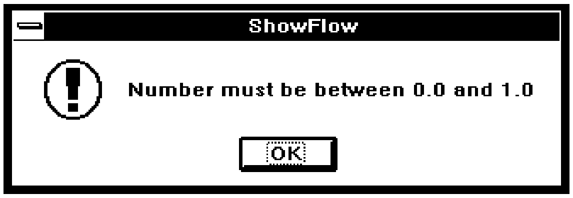
To *select* an entire word or numeric entry, simply double-click on the entry with the mouse or drag the mouse (holding down the button) across the desired selection. Selected text appears in reverse video. Any typing done now will replace the selected text. If you do not want to replace the text but rather edit it, use the mouse or the arrow keys to position the cursor in the box. The DELETE key will delete to the right of the cursor, and the BACKSPACE key to the left.

③ Move to the other text fields beside each parameter description with either the mouse or the TAB key. (To move backwards, use SHIFT + TAB.) Edit the contents of each window as desired.

④ *Radio buttons* ○ are used to choose among mutually exclusive options which appear in various dialog boxes. Depending on the choice made, some entry fields may be disabled or enabled as appropriate. Radio buttons are chosen by either clicking with the mouse, or using the ↑ and ↓ keys to move and the SPACEBAR to select.

⑤ *Check boxes* ☐ are used to enable or disable non-exclusive options. These are also selected with the SPACEBAR.

⑥ Accept the new values by choosing the "OK" pushbutton (ENTER). "Cancel" (ESC) will abandon any changes made.



Number must be between 0.0 and 1.0

Figure 18 An example of a data entry error message

The Hydrologic Parameters, Hydrocarbon Phase Parameters and Simulation Parameters dialog boxes contain a check box titled "Enable range checking." This box is normally checked and causes HSSM-WIN to check each parameter to assure that it is within allowable limits. Each field will be tested for illegal characters or out-of-range values, in which case an error message will appear as in **Figure 18**. After acknowledging this message with "OK," the user will have the opportunity to edit the offending field where HSSM-WIN has moved the prompt. Disabling the range checking option causes HSSM-WIN not to check the parameter values.

⑦ After exiting the editing dialog box, the changes are in HSSM-WIN's memory, but *they are not yet saved to a file*. Use the "Save" or "SaveAs" commands to save them.

NOTE: To view the underlying graphs while assigning values to the parameters, the Editing window (like any other) can be almost entirely moved off the screen by dragging its title bar.

4.6.2 Required Units for HSSM Simulations

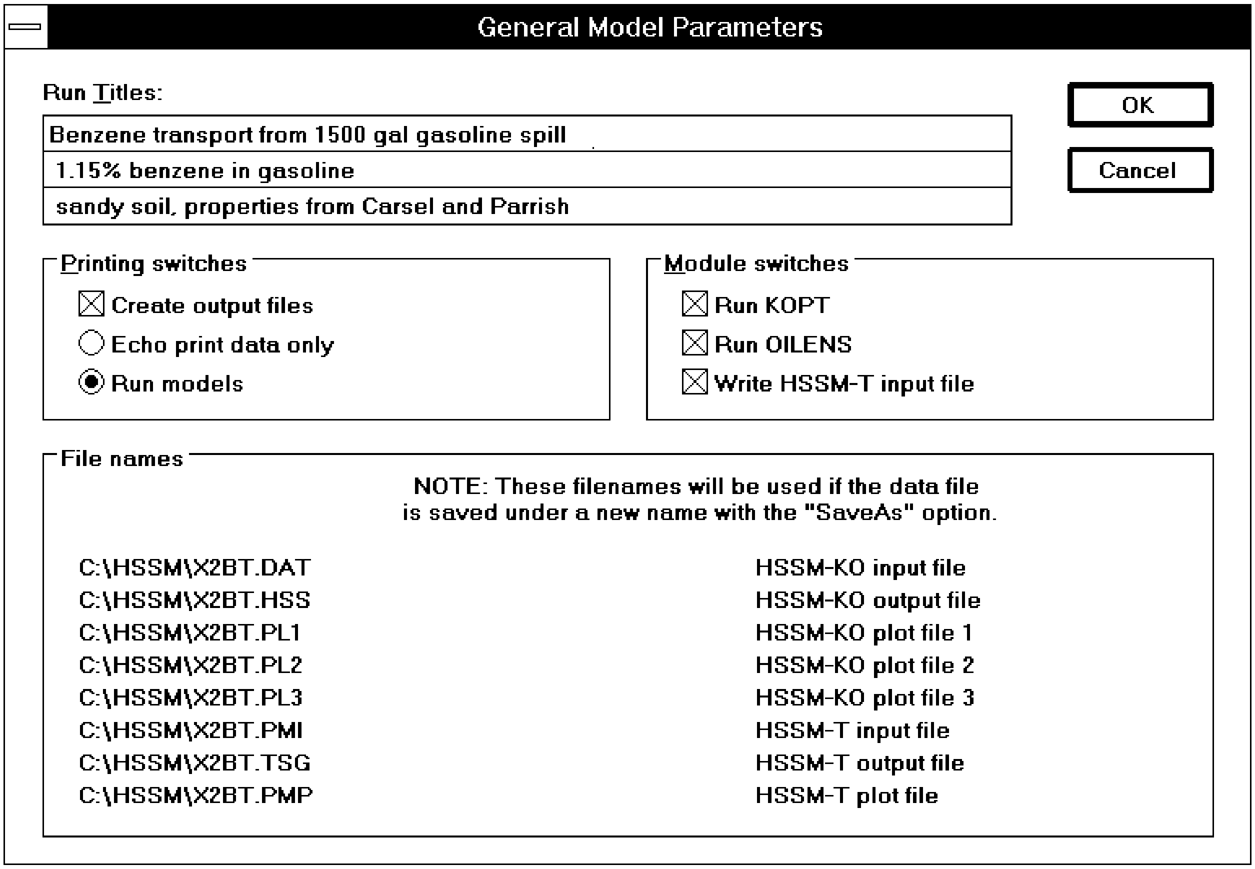
The following units are used in HSSM and are listed with their usage and abbreviation. Care must be taken to assure that all input parameters are converted to this set of units. As a reminder, the required units are listed with each parameter discussed below.

Table 8 Required Units for HSSM Simulations

Quantity	Unit
Time	day
Depth	meter
Dynamic Viscosity	centipoise
Density	grams/cubic centimeter
Surface Tension	dyne/centimeter
Concentration	milligrams/liter
Soil-Water Partition Coefficient	liters/kilogram
Dispersivity	meters
Various	dimensionless

4.6.3 General Model Parameters

The **General Parameters** dialog box (**Figure 19**) contains titles, printing switches, module switches, and file names.



Run Titles:

Benzene transport from 1500 gal gasoline spill

1.15% benzene in gasoline

sandy soil, properties from Carsel and Parrish

Printing switches

☒ Create output files

○ Echo print data only

● Run models

Module switches

☒ Run KOPT

☒ Run OILENS

☒ Write HSSM-T input file

File names

NOTE: These filenames will be used if the data file
is saved under a new name with the "SaveAs" option.

C:\HSSM\X2BT.DAT	HSSM-KO input file
C:\HSSM\X2BT.HSS	HSSM-KO output file
C:\HSSM\X2BT.PL1	HSSM-KO plot file 1
C:\HSSM\X2BT.PL2	HSSM-KO plot file 2
C:\HSSM\X2BT.PL3	HSSM-KO plot file 3
C:\HSSM\X2BT.PMI	HSSM-T input file
C:\HSSM\X2BT.TSG	HSSM-T output file
C:\HSSM\X2BT.PMP	HSSM-T plot file

Figure 19 General Parameters dialog box

Run Titles

A three-line run title is used by HSSM-WIN. These text strings are included in all of the output and plot files. The first line is also used as a graph title. If the graph is too small to plot, the graph window contains only the three title lines.

Printing switches

☐ **Create output files**

If this switch is chosen, output files will be generated by the models. The normal situation is to choose this option.

○ **Echo print data only**

○ **Run Models**

This switch tells the model either to run and create plot files, or only to echo the input data. Echo printing, to check the input file, is recommended before making the simulation run.

Module switches

☐ **Run KOPT**

Run the KOPT module of HSSM-KO. KOPT simulates the infiltration of the NAPL through the vadose zone. KOPT must be run in order to run OILENS or TSGPLUME.

☐ Run OILENS

Run the OILENS module of HSSM-KO, to simulate the motion and dissolution of the hydrocarbon lens at the water table. OILENS requires that KOPT also be run.

☐ Write TSGPLUME input file

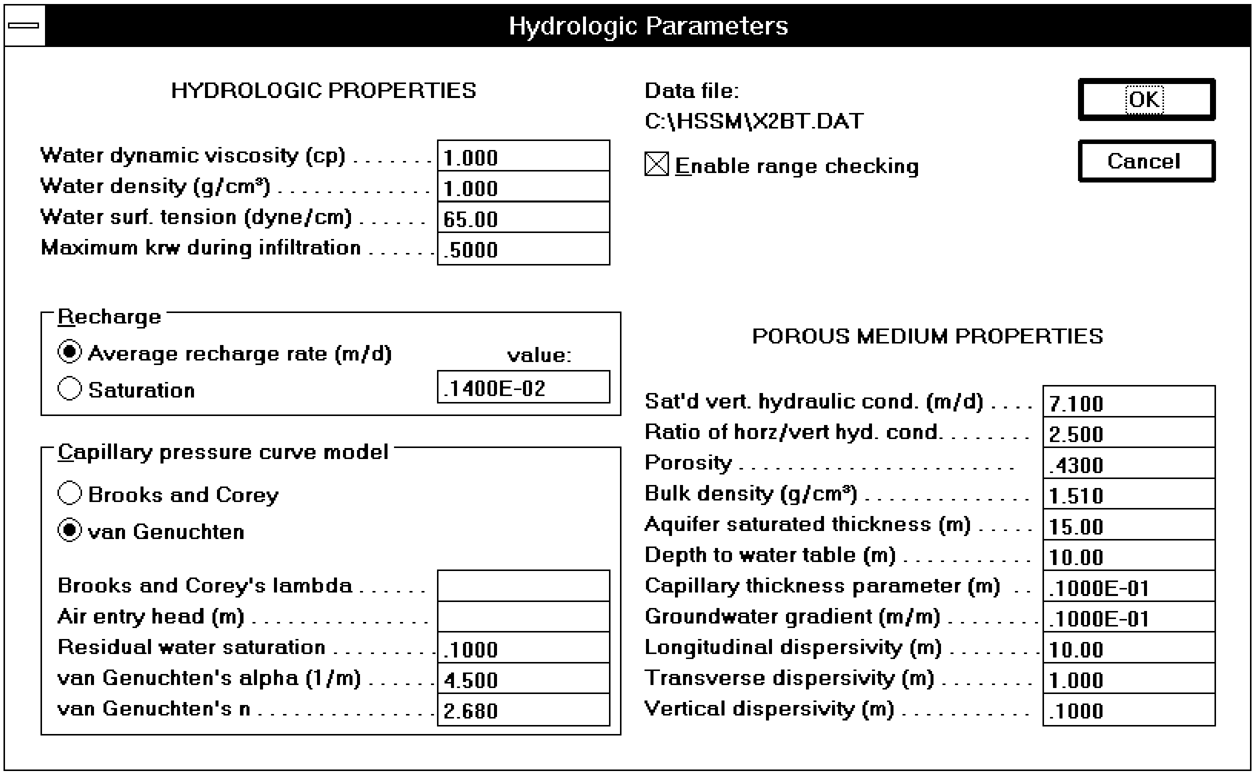
Write the TSGPLUME (HSSM-T) input data file when the HSSM-KO program is run. This option must be selected if HSSM-T is to be run. HSSM-T, which simulates transport of the chemical constituent in the aquifer, is run using the "Run HSSM-T" command, only after HSSM-KO has run.

File names

HSSM requires the use of a specific set of files for producing output and plot files. These names can not be edited, but are included for the user's information as they will appear in the indicated directory after running the model. The names change automatically whenever the file is saved under a new name. The names and purposes of the files are listed in section 4.7.

4.6.4 Hydrologic and Hydraulic Data

The **Hydrologic Parameters** dialog box (**Figure 20**) lists hydrologic and hydraulic data for the model.



HYDROLOGIC PROPERTIES

Water dynamic viscosity (cp) 1.000
Water density (g/cm^3) 1.000
Water surf. tension (dyne/cm) 65.00
Maximum krw during infiltration ...... .5000

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

Recharge
● Average recharge rate (m/d)
○ Saturation
value: .1400E-02

Capillary pressure curve model
○ Brooks and Corey
● van Genuchten

Brooks and Corey's lambda ......
Air entry head (m) ....
Residual water saturation .... .1000
van Genuchten's alpha (1/m) 4.500
van Genuchten's n 2.680

POROUS MEDIUM PROPERTIES

Sat'd vert. hydraulic cond. (m/d) 7.100
Ratio of horz/vert hyd. cond. 2.500
Porosity .... .4300
Bulk density (g/cm^3) 1.510
Aquifer saturated thickness (m) 15.00
Depth to water table (m) 10.00
Capillary thickness parameter (m) .. .1000E-01
Groundwater gradient (m/m) .... .1000E-01
Longitudinal dispersivity (m) 10.00
Transverse dispersivity (m) 1.000
Vertical dispersivity (m) .... .1000

Figure 20 Hydrologic Parameters dialog box

HYDROLOGIC PROPERTIES

Water dynamic viscosity, μ_w (cp)

Enter the dynamic viscosity of water in centipoise (cp). At 20° C the viscosity of pure water is 1.0 cp.

Water density, ρ_w (g/cm^3)

Enter the density of water in g/cm^3. At 20° C the density of pure water is 1 g/cm^3.

Water surface tension, σ_{aw} (dyne/cm)

Enter the water/air surface tension in dyne/cm. At 20° C the surface tension of pure water is 72.8 dyne/cm. A lower value, say 65 dyne/cm, may be appropriate for soils and/or contaminated sites.

Maximum relative permeability to water, $k_{rw(max)}$, during infiltration

Enter the maximum water relative permeability during infiltration. Since air is normally trapped during infiltration, the effective hydraulic conductivity of the soil will be less than the saturated conductivity. The relationship between effective conductivity to water, K_{ew}, and saturated conductivity to water, K_{sw} is given by

$$K_{ew} = K_{sw} k_{rw} \qquad \textbf{(1)}$$

where k_{rw} is called the relative permeability to water. The relative permeability equals zero when the saturation is at or below residual, and equals one when the porous medium is completely saturated with water.

To account for trapping of the air phase, the maximum effective conductivity is restricted by the value set for $k_{rw(max)}$. Typical values range from 0.4 to 0.6 (Bouwer 1966); 0.5 is often used (e.g., Brakensiek et al., 1981). The maximum water saturation is then determined from the k_{rw} function that is used by HSSM. The remainder of the pore space is assumed to be filled with trapped air. The water saturation calculated from $k_{rw(max)}$ is then discarded, as only the trapped air saturation is used by the model.

Recharge

Check the type of recharge condition desired. Recharge can as either by specifying a recharge rate or as a vadose zone residual water saturation.

○ Average annual recharge rate, q_w (m/d)

Choose this option to specify a recharge flux.

○ Saturation, $S_{w(max)}$

Choose this option to specify a constant water saturation in the pore space.

When annual recharge is chosen for the recharge input:

The value entered is the average annual recharge rate. For example, with an annual recharge rate of 10 cm/yr the value entered is:

$$2.74 \times 10^{-4} \frac{m}{d} = 10 \frac{cm}{yr} \left(\frac{m}{100\, cm} \right) \left(\frac{yr}{365\, d} \right) \qquad \textbf{(2)}$$

HSSM-KO calculates the water saturation (fraction of the pore space that is filled with water) from the recharge rate. Large recharge rates may cause the available pore space to be completely filled with water, allowing no NAPL to infiltrate. If such conditions are encountered an error message is written to the screen.

When saturation is chosen for the recharge input:

If 35% of the pore space is filled by water, then 0.35 is entered here. Using the other set of units: if the volumetric moisture content is 0.14 and the porosity is 0.40, then the equivalent saturation of 0.35 is entered here.

Typically the moisture content at or above the *field capacity* would be used here, after converting to saturation. The relationship between volumetric moisture content, θ_w, porosity, η, and saturation, S_w, is given by $\theta_w = \eta S_w$. From the saturation input, HSSM-KO calculates the associated water flux.

Capillary Pressure Curve Model

○ **Brooks and Corey**
○ **van Genuchten**

Choose the capillary pressure model to be used in HSSM calculations. Further information on the selection of the model parameters is given in Appendix 3.1 "Soil Properties." Either Brooks and Corey or van Genuchten model parameters may be used. The appendix contains typical parameter values for each of these models. Although the HSSM is designed to use the Brooks and Corey model, van Genuchten model parameters may be entered as input. The van Genuchten model parameters are converted to approximately equivalent Brooks and Corey model parameters by a procedure developed by Lenhard et al. (1989). Only the parameters highlighted for the chosen model need be entered.

For the Brooks and Corey Model:

The Brooks and Corey (1964) model equation which describes the relationship between saturation S_w and capillary head h_c is given by

$$\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right) = \left(\frac{h_{ce}}{h_c}\right)^{\lambda} \tag{3}$$

where the residual water saturation, S_{wr}, the air entry head, h_{ce}, and the pore size distribution index, λ, are fitting parameters.

Brooks & Corey's λ

The parameter λ is called the pore size distribution index, and is determined by either fitting the Brooks and Corey model to the water/air capillary pressure curve $P_c(S_w)$ by a procedure outlined by Brooks and Corey (1964), or by non-linear curve fitting (e.g., van Genuchten et al., 1991).

Brooks & Corey's Air entry head, h_{ce} (m)

Enter the absolute value of the air entry head in meters. This value is determined as a parameter from the water/air capillary pressure curve (see item on Brooks and Corey's λ, above.)

Residual water saturation, S_{wr}

Enter the residual water saturation, which is determined from the measured capillary pressure curve (see item on Brooks and Corey's λ, above.)

For the van Genuchten Model:

NOTE: selecting the van Genuchten model causes HSSM to calculate approximately equivalent Brooks and Corey model parameters as described in Appendix 4.

van Genuchten's model is defined by

$$\frac{\theta_w - \theta_{wr}}{\theta_m - \theta_{wr}} = \frac{1}{\left[1 + (\alpha h_c)^n\right]^m} \tag{4}$$

where

θ_w = volumetric water content

h_c = capillary head with units of m
θ_{wr} = volumetric residual water content
θ_m = volumetric maximum water content
α = a parameter with units of m^{-1}
n = a parameter
m = a parameter (taken as a simple function of n)

For HSSM the reduced water content term (the left hand side of van Genuchten's model) is taken to be equal to

$$\frac{S_w - S_{wr}}{1 - S_{wr}} \tag{5}$$

where the maximum water saturation, θ_m, has been equated with the porosity. The parameters of van Genuchten's model can be fitted to measured data by using a fitting program like RETC (van Genuchten et al., 1991).

Residual water saturation, S_{wr}

Enter the residual water saturation, which is determined from the measured capillary pressure curve.

van Genuchten's α

Enter the value of van Genuchten's parameter α in units of m^{-1}.

van Genuchten's n

Enter the value of van Genuchten's parameter n.

POROUS MEDIUM PROPERTIES

Saturated vertical hydraulic conductivity, K_s (m/d)

Enter the value of the saturated vertical water phase hydraulic conductivity, K_s, in meters per day. Saturated hydraulic conductivity is one of the most important parameters of the model. Estimation of this parameter is described in Appendix 3.1 "Soil Properties." This appendix contains data from two tabulations of soil properties.

Ratio of horizontal to vertical hydraulic conductivity

Enter the ratio of the horizontal saturated water phase conductivity to the saturated vertical water phase hydraulic conductivity. Anisotropy is not treated directly in HSSM, rather the model uses the product of the ratio RKS and the saturated vertical conductivity, K_s, to determine the hydraulic conductivity of the aquifer. This later conductivity is also used for determining the effective conductivity to the NAPL for the lens spreading. The relationships between the conductivities are summarized in Table 9.

Table 9 Summary of Hydraulic Conductivity Relationships

Model and Region	Hydraulic Conductivity Used	HSSM Variables
Vadose zone (KOPT)	Vertical	K_s
NAPL lens (OILENS)	Horizontal	K_s*RKS
Aquifer (TSGPLUME)	Horizontal	K_s*RKS

Porosity, η

Enter the porosity, η, of the aquifer.

Bulk density, ρ_b (g/cm^3)

Enter the bulk density of the soil in g/cm^3. Porosity, η, and bulk density, ρ_b are related by

$$\rho_b = \rho_s(1 - \eta) \tag{6}$$

where ρ_s is the solids density. The density of quartz is approximately 2.65 g/cm^3. The values for porosity and bulk density must be related by equation **(6)**.

Aquifer saturated thickness (m)

Enter the saturated thickness of the aquifer in meters.

Depth to water table (m)

Enter the depth to the water table from the release point in meters. The release point is usually at the ground surface.

Capillary thickness parameter (m)

The capillary thickness parameter gives the model a thickness which must build up in the capillary fringe before spreading of the NAPL occurs. Typically, a value of 0.01m should be entered for this parameter. This results in a small thickness of NAPL that is built up before spreading begins.

The capillary thickness parameter can also be used to incorporate the effect of water table fluctuation on the lens radius. Water table fluctuation can cause trapping of NAPL throughout a smear zone, and the trapped NAPL is not available for radial spreading. To include this effect, the capillary thickness parameter should be calculated by

$$\begin{pmatrix} \textit{capillary} \\ \textit{thickness} \\ \textit{parameter} \end{pmatrix} = \frac{\textit{smear zone thickness} \times \textit{residual NAPL saturation}}{\textit{maximum NAPL saturation in lens}} \qquad \textbf{(7)}$$

The smear zone thickness should be taken as the maximum water table fluctuation. The residual NAPL saturation and maximum NAPL saturation in the lens are described under the Hydrocarbon Phase Data dialog box (Section 4.6.5).

Ground water gradient (m/m)

Enter the ground water gradient. Typical maximum natural gradients range from 0.005 to 0.02. Since pumping wells are not allowed in TSGPLUME, natural gradients should be used here.

Aquifer Dispersivities A_L, A_T, A_V (m): Longitudinal, Horizontal Transverse, Vertical Transverse.

Enter the longitudinal, horizontal transverse and vertical transverse dispersivities in meters. The dispersivities are defined by

$$\begin{aligned} D_L &= A_L\, v \\ D_T &= A_T\, v \\ D_V &= A_V\, v \end{aligned} \qquad \textbf{(8)}$$

where D_L, D_T, and D_V are the longitudinal, horizontal transverse, and vertical transverse dispersion coefficients; A_L, A_T, and A_V are likewise the longitudinal, horizontal transverse, and vertical transverse dispersivities; and v is the seepage velocity in the mean flow direction.

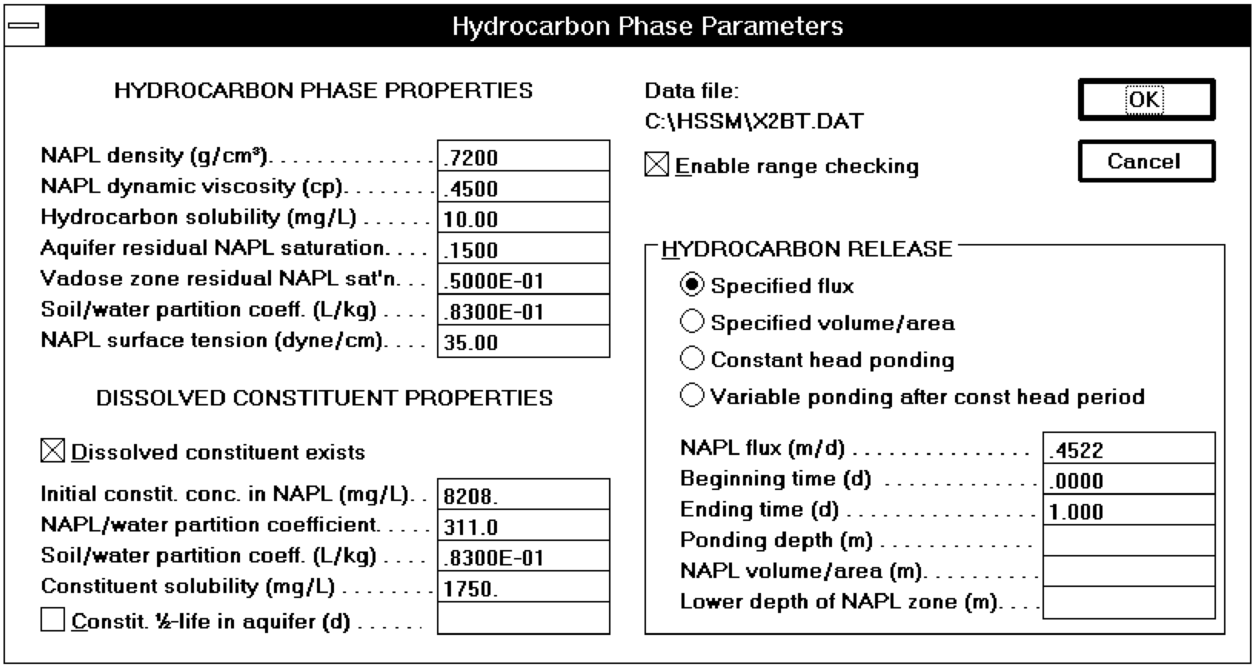
Dispersive mixing in aquifers results from solute transport through heterogeneous porous media. As the contaminant plume spreads it "experiences" more heterogeneity and the apparent dispersion coefficient increases. Thus the dispersion coefficients, D_L, D_T and D_V are not fundamental parameters, but exhibit scale dependence.

Gelhar et al. (1992) recently reviewed dispersivities determined at 59 sites and considered the reliability of the dispersion coefficients. They concluded that there are no highly reliable longitudinal dispersion coefficients at scales greater than 300m. Notably, at a given scale, dispersivities have been found to vary by 2 to 3 orders of magnitude, although the lower values are more reliable.

Based on these data, horizontal transverse dispersivities are typically from 1/3 to almost 3 orders-of-magnitude lower than longitudinal dispersivities. Vertical transverse dispersivities are typically (although based on a very limited data set) 1-2 orders-of-magnitude lower than horizontal transverse dispersivities. The very low values of vertical transverse dispersivities reflect roughly horizontal stratification of sedimentary materials.

4.6.5 Hydrocarbon (NAPL) Phase Data

The **Hydrocarbon (NAPL) Phase Parameters** dialog box (**Figure 21**) contains data concerning the nature of the spilled hydrocarbon and one constituent of interest.



HYDROCARBON PHASE PROPERTIES

NAPL density (g/cm³)	.7200
NAPL dynamic viscosity (cp)	.4500
Hydrocarbon solubility (mg/L)	10.00
Aquifer residual NAPL saturation	.1500
Vadose zone residual NAPL sat'n.	.5000E-01
Soil/water partition coeff. (L/kg)	.8300E-01
NAPL surface tension (dyne/cm)	35.00

DISSOLVED CONSTITUENT PROPERTIES

☒ Dissolved constituent exists

Initial constit. conc. in NAPL (mg/L)	8208.
NAPL/water partition coefficient	311.0
Soil/water partition coeff. (L/kg)	.8300E-01
Constituent solubility (mg/L)	1750.
☐ Constit. ½-life in aquifer (d)	

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

HYDROCARBON RELEASE

● Specified flux
○ Specified volume/area
○ Constant head ponding
○ Variable ponding after const head period

NAPL flux (m/d)	.4522
Beginning time (d)	.0000
Ending time (d)	1.000
Ponding depth (m)	
NAPL volume/area (m)	
Lower depth of NAPL zone (m)	

Figure 21 Hydrocarbon Phase Parameters dialog box

HYDROCARBON PHASE PROPERTIES

NAPL density, ρ_o (g/cm^3)

Enter the NAPL phase density in g/cm^3. For OILENS simulations, the NAPL density must be less than that of water. Densities greater than water may be used if no OILENS simulation is performed. Some typical NAPL densities are given in Table 10.

Hydrocarbon densities are sometimes expressed by the degrees API (Perry and Chilton, 1973) scale adopted by the American Petroleum Institute. Degrees API is defined by

$$^\circ API \quad = \quad \frac{141.5}{sp.gr.} - 131.5 \qquad \textbf{(9)}$$

where sp.gr. is the specific of the NAPL measured at 70° F divided by the specific gravity of water measured at 60° F. The degrees API scale runs from 0.0 to 100.0 and covers a range of specific gravities from 1.076 to 0.6112.

NAPL dynamic viscosity, μ_o (cp)

Enter the NAPL phase viscosity in centipoise. Typical NAPL viscosities are given in Table 10.

The densities and viscosities of the NAPL and water phases are used by HSSM-KO to estimate the saturated hydraulic conductivity to the NAPL phase, K_{so}, by

$$K_{so} = K_{sw} \frac{\mu_w}{\mu_o} \frac{\rho_o}{\rho_w} \qquad \textbf{(10)}$$

where K_{sw} is the saturated hydraulic conductivity to water, μ_w and μ_o are the water and oil viscosities, and ρ_w and ρ_o are the respective densities.

Table 10 NAPL Densities and Viscosities at 20°C

Liquid	Density g/cm_3	Viscosity Cp
Methylene Chloride	1.33	0.426
TCE	1.47	0.566
PCE	1.60	0.900
Gasoline	0.75	0.45
Carbon Tetrachloride	1.59	0.970
Water	1.00	1.00
No. 2 Fuel Oil	0.87	5.9
Transmission Fluid	0.89	80
Aroclor 1254	1.51	2050

Hydrocarbon (NAPL) solubility (mg/L)

Enter the NAPL water solubility in mg/L. This coefficient represents the solubility of all of the NAPL constituents, except the chemical constituent that is simulated. The solubility of the chemical constituent is entered separately. Further, this value is only used by the model in a substantial way if one particular ending criterion is used. Therefore the value of the NAPL solubility is not a critical parameter.

The value of NAPL solubility must be greater than zero if the **OILENS Simulation ending criterion** (see below) is set to ② "NAPL lens spreading stops." Bauman (1989) estimated that the typical solubility of gasoline is on the order of 50 to 200 mg/L.

Aquifer residual NAPL saturation, S_{ors}

Enter the residual NAPL phase saturation in the aquifer. See notes below for the vadose zone residual NAPL saturation.

Vadose zone residual NAPL saturation, S_{orv}

Enter the residual NAPL phase saturation for the vadose zone. By definition, the NAPL phase does not flow at saturations less than or equal to residual. In this model, the residual NAPL saturation is assumed to be a known constant. Ideally, this would be obtained by measuring the NAPL/air capillary pressure curve in the presence of the amount of water filling a portion of the pore space. Treating the residual NAPL saturation as a constant is acknowledged to be an assumption, as in actuality the NAPL residual saturation may vary with the hydraulic gradient and with time as the NAPL weathers (Wilson and Conrad, 1984.) Typically the residual NAPL saturation in the vadose zone is less than that for the aquifer (with the same media properties). Typical hydrocarbon residual saturations vary from 0.10 to 0.20 in the vadose zone, and from 0.15 to 0.50 in the saturated zone (Mercer and Cohen, 1990). These values correspond more closely to "specific retention", as the term is used in ground water hydrology, rather than true residuals at large capillary pressure values.

Soil/water partition coefficient (L/kg)

Enter the linear equilibrium partitioning coefficient between the soil and the water phase concentrations (c_s and c_w) of the hydrocarbon phase. Like the solubility of the NAPL phase, listed above, this parameter is not critical. This coefficient is used for estimating the partitioning of the dissolved fractions of the NAPL (i.e., all of the NAPL chemicals except the chemical constituent of interest). For further information on partitioning see the discussion below for the constituent soil/water partition coefficient.

NAPL surface tension, σ_{ao} (dyne/cm)

Enter the NAPL surface tension in dyne/cm. Table 11 shows typical surface tension values for several petroleum products

Table 11 Surface tensions of several fuels (Wu and Hottel, 1991)

Liquid	Surface tension (dyne/cm)
gasoline	26
kerosene	25-30
gas oil	25-30
lubricating fractions	34
fuel oils	29-32

DISSOLVED CONSTITUENT PROPERTIES

☐ Dissolved constituent exists

Check this box if calculations are to be performed for a dissolved constituent. Normally, for full HSSM transport simulation to a receptor point this will be checked.

Initial constituent concentration in the NAPL, $c_{o(ini)}$ (mg/L)

Enter the initial concentration of dissolved chemical in the NAPL phase in mg/L. HSSM idealizes the multiphase/multicomponent system as consisting of a NAPL phase that contains some small fraction of a dissolved constituent. The dissolved constituent can partition between the fluids and the solid. The concentration of the chemical in the NAPL is entered here. For example, benzene composes 1.14% by mass of the idealized gasoline mixture used by Baehr & Corapcioglu (1987). The initial benzene (the chemical constituent) concentration in gasoline (the NAPL or "oil") is given by

$$C_b = f_b \rho_g \qquad \textbf{(11)}$$

where C_b is the concentration of benzene in the gasoline, f_b is the mass fraction of benzene in gasoline, ρ_g is the density of the gasoline. Therefore

$$C_b\,(g/cm^3) = \frac{1.14\%}{100}\,(0.73\,g/cm^3) = 0.0083\,g/cm^3 \qquad \textbf{(12)}$$

Converting the gasoline concentration to the required units gives

$$C_b\,(mg/L) \;=\; C_b\,(g/cm^3)\;\left(\frac{1000\;\; cm^3}{L}\right)\;\left(\frac{1000\;\; mg}{g}\right) \;=\; 8300\,mg/L \qquad \textbf{(13)}$$

NAPL/water partition coefficient, K_o

Enter the linear equilibrium partitioning coefficient between the NAPL and the water phase concentrations of the chemical constituent. By definition

$$c_o \;=\; K_o\; c_w \qquad \textbf{(14)}$$

where K_o is the dimensionless partition coefficient between the NAPL phase (c_o) and water phase (c_w) concentrations of the chemical constituent. The partitioning between the NAPL phase and the water phase depends on the composition of the NAPL. Estimation of K_o is discussed in Appendix 3.2 "NAPL/Water Partition Coefficient." A utility program for performing the necessary calculations, called RAOULT, is described in Appendix 6.

Soil/water partition coefficient, K_d (L/kg)

Enter the linear equilibrium partitioning coefficient in liters per kilogram between the soil and the water phase concentrations (c_s and c_w) of the constituent. By definition

$$c_s \;=\; K_d\; c_w \qquad \textbf{(15)}$$

where K_d is the partition coefficient in liters per kilogram between the solid (c_s) and water phase concentrations (c_w). K_d is commonly estimated from the fraction organic carbon of the media, f_{oc}, and the organic carbon partition coefficient, K_{oc} as

$$K_d \;=\; f_{oc}\, K_{oc} \qquad \textbf{(16)}$$

(44) in Appendix 3 lists K_{oc} values for several hydrocarbons.

Constituent solubility, s_k (mg/L)

Enter the chemical constituent water solubility in mg/L. The solubility entered here is the "pure component" solubility which is tabulated in several sources (i.e., Mercer et al., 1990; Sims et al., 1991; USEPA, 1990). Several values are given in Table 98. The solubility is used by HSSM to limit the water phase concentration. Appropriately chosen K_o values (which imply maximum water phase concentrations much less than the pure phase solubilities) make this parameter redundant for NAPLs composed of mixtures of chemicals.

☐ Constituent half-life in aquifer (d)

Enter the half-life of the constituent in the aquifer and check the box. If the box is not checked, HSSM-WIN passes a very large value to the model, causing there to be no decay in the TSGPLUME model. This value is used only by the TSGPLUME model.

HYDROCARBON (NAPL) RELEASE

The Hydrocarbon Release box defines, in part, the boundary condition for the simulation. Four options are provided for specifying the way in which the NAPL enters the subsurface. Not all of the release parameters are needed for each release option; the necessary parameters for the selected option are highlighted by HSSM-WIN for entry of the specific values.

Release Options

○ Specified flux

Specifies a constant flux of NAPL, corresponding to a known rate of application of NAPL to the ground surface for a specified time interval. Excess NAPL is assumed to run off at the surface.

○ Specified volume/area

Specifies a volume per unit area of NAPL applied over a certain depth. This results in a fixed volume applied instantaneously, corresponding to a land treatment system or a landfill.

○ Constant head ponding

Specifies constant head ponding for a specified duration. The ponding depth abruptly goes to zero at the end of the release. This condition is used to simulate a hydrocarbon tank rupture which is contained within a berm, for example.

○ Variable ponding after a period of constant head ponding

Specifies constant head ponding for a specified duration, followed by a gradual decrease to zero head as the NAPL infiltrates.

Release Parameters

NAPL flux, q_o (m/d)

Enter the constant NAPL flux in meters per day. NAPL phase fluxes in excess of the maximum effective oil phase conductivity are assumed to run off.

Beginning time (d)

Enter the beginning time of the NAPL release in days. Usually this is zero.

Ending time (d)

Enter the ending time of the NAPL release in days or the ending time of constant head ponding.

Ponding depth, H_s (m)

Enter the depth of constant head ponding in meters.

Oil volume/area (m^3/m^2) or (m)

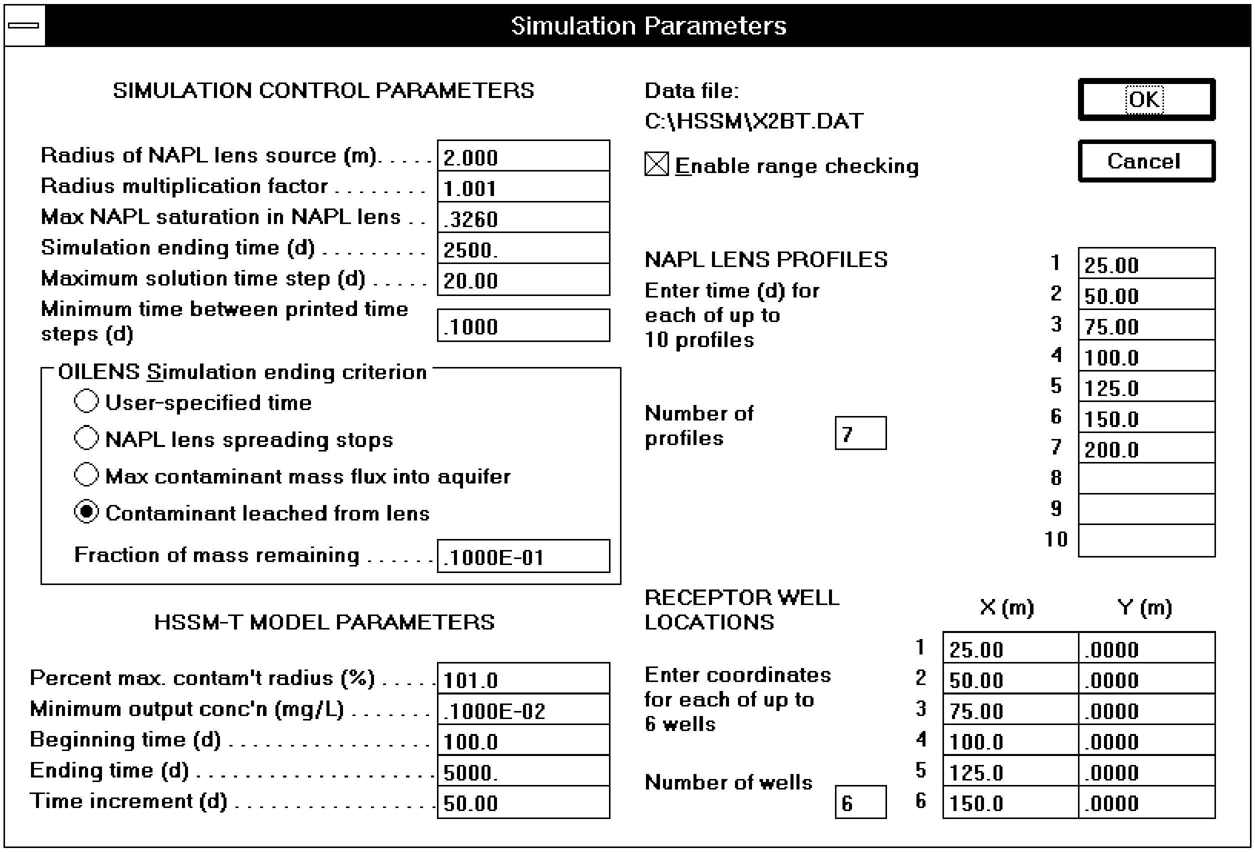
Enter the volume of the NAPL phase per unit surface area that is placed in either a land treatment facility or a landfill.

Lower depth of NAPL zone (m)

Enter the depth of the bottom of the contaminated zone in meters.

4.6.6 Model Simulation Data

The **Model Simulation Parameters** dialog box (**Figure 22**) contains data controlling the simulations, such as beginning and ending times, numbers and locations of wells, etc.



SIMULATION CONTROL PARAMETERS

Radius of NAPL lens source (m)	2.000
Radius multiplication factor	1.001
Max NAPL saturation in NAPL lens	.3260
Simulation ending time (d)	2500.
Maximum solution time step (d)	20.00
Minimum time between printed time steps (d)	.1000

OILENS Simulation ending criterion

○ User-specified time
○ NAPL lens spreading stops
○ Max contaminant mass flux into aquifer
● Contaminant leached from lens

Fraction of mass remaining: .1000E-01

HSSM-T MODEL PARAMETERS

Percent max. contam't radius (%)	101.0
Minimum output conc'n (mg/L)	.1000E-02
Beginning time (d)	100.0
Ending time (d)	5000.
Time increment (d)	50.00

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

NAPL LENS PROFILES

Enter time (d) for each of up to 10 profiles

Number of profiles: 7

1	25.00
2	50.00
3	75.00
4	100.0
5	125.0
6	150.0
7	200.0
8	
9	
10	

RECEPTOR WELL LOCATIONS

Enter coordinates for each of up to 6 wells

Number of wells: 6

	X (m)	Y (m)
1	25.00	.0000
2	50.00	.0000
3	75.00	.0000
4	100.0	.0000
5	125.0	.0000
6	150.0	.0000

Figure 22 Model Simulation Data dialog box

SIMULATION CONTROL PARAMETERS

Radius of oil lens source, R_s (m)

Enter the radius of the contaminant source in meters. When no OILENS simulation is desired (Run OILENS is not selected on the General Model Parameters dialog box), a *per unit area* simulation can be performed by entering 0.5642 as the radius of the source. The resulting source area is 1.0 m^2.

Radius multiplication factor

A value of 1.001 is suggested for the radius multiplication factor (RMF). The RMF is used to multiply the source radius for starting the OILENS model. This is necessary since the OILENS equations are singular at the source radius. Starting the simulation at a small distance from the true radius avoids this singularity. This procedure does, however, introduce a mass balance error into the solution, so the minimum value of RMF which permits the simulation to proceed should be used. At no time should the RMF exceed 1.1. When the singularity is encountered, the OILENS model will display the error message

```
OILENS SINGULARITY ENCOUNTERED, INCREASE RMF.
```

The RMF should then be increased, and the simulation retried.

Maximum NAPL saturation in the NAPL lens, $S_{o(max)}$

Enter the saturation of the NAPL phase in the lens. In HSSM, the lens is idealized as a uniformly saturated lens, although in actuality the NAPL saturation varies within the lens. The thickness of the lens in HSSM represents the ratio of the volume of the lens to its area. Estimation of the NAPL lens saturation is discussed in Appendix 3.3, and a utility called NTHICK for performing the necessary calculation is described in Appendix 7.

Simulation ending time (d)

Enter the simulation ending time in days. This must always be specified, even though other stopping options are available and may override the maximum simulation time.

Maximum solution time step (d)

Enter the maximum solution time step in days. This should be set as high as possible, although internal error correction routines will often limit the actual size of the step taken. Values of up to 25 days are usually acceptable. Overly large step sizes may introduce mass balance errors in the model results.

Minimum time between printed time steps and mass balance checks (d)

Enter the minimum time between printed time steps in days. Although the model uses a variable time step ordinary differential equation solver, at times during the simulation HSSM takes very small steps. Results from these steps are of little use and dramatically increase the size of the output files. This parameter prevents the output of every solution step and should be set to 0.1 or 0.25 days. This parameter does not affect the simulation itself, but only the information that is output.

For most chemicals leaching out of the lens, after the peak mass flux into the aquifer has passed, there is a relatively long period of time where the mass flux into the aquifer slowly declines. During this time period, the user-set minimum time between printed time steps may be overridden in order to reduce the size of the output and plot files. An additional criterion is added that the mass flux must change by at least 1.0 percent for the results to be output. This feature cannot be overridden by the user.

OILENS simulation ending criterion

The OILENS Simulation ending criterion determines how the HSSM-KO simulation terminates. Because it is not possible to predict when certain events in the simulation will occur, several of the options cause the simulation to end only after the event of interest has occurred. In these cases the user-specified ending time is overridden and the simulation continues until the event occurs.

NOTE: The fourth option, "Contaminant leached from lens" must be chosen in order to use the HSSM-T model.

① User-specified time

Stop at the simulation ending time specified above.

② NAPL lens spreading stops

Stop the simulation when the NAPL lens stops spreading. If no NAPL lens forms before the specified ending time, then the simulation stops at the specified ending time. If a lens does form, the ending time is overridden and the simulation continues until the NAPL lens stops spreading. When the NAPL phase solubility is near zero, it is possible that, in the model, the lens motion may never stop, since kinematic theory predicts that an infinite amount of time is required for all of the NAPL to pass a given depth. The NAPL trickles into the lens throughout the simulation, and NAPL lens motion stops when the flux into the lens drops below the NAPL dissolution flux into the aquifer. If the NAPL solubility is zero and no chemical constituent is simulated, no NAPL is dissolved and the motion may continue indefinitely. To avoid this problem, *a non-zero NAPL solubility* (see Hydrocarbon Phase Parameters) is required for this situation.

③ Maximum contaminant mass flux into aquifer

Stop the simulation when the maximum chemical constituent flux into the aquifer occurs. If no NAPL lens forms before the specified ending time, the simulation stops at the specified ending time. If a lens forms, the ending time is overridden and the simulation continues until the maximum mass flux occurs.

④ Contaminant leached from lens drops below a given fraction of the total mass in the lens

Stop the simulation when the contaminant mass in the NAPL lens drops below a specified fraction of the maximum contaminant mass that has been contained within the lens during the entire simulation. The fraction is specified by the user. If no NAPL lens forms before the user-specified ending time (above), the simulation stops at the specified ending time.

Fraction of mass remaining

Enter the mass factor stopping criterion for the above ending criterion ④ "Contaminant leached from lens". Two percent (0.02) or less should be used for this factor.

TSGPLUME MODEL PARAMETERS

The following parameter values are used by the TSGPLUME model only.

Percent maximum contaminant radius (%)

Enter the percentage of the maximum contaminant radius which is to be used in the TSGPLUME simulation, which requires a constant radius for the input mass flux.

Since the radius of the NAPL lens changes continuously during part of the simulation, it may not be possible to preselect an appropriate lens radius for the TSGPLUME module. It is desirable, however, to match the radius of the lens to the peak mass flux into the aquifer. Thus TSGPLUME simulation can use the radius which occurs at the time of the maximum mass flux. With this approach the peak mass flux is not overly diluted due to a large lens radius. (Nor is it "condensed" due to an overly small radius). The lens radius which occurs at the time of the maximum mass flux is automatically selected if 101 is entered for the percent maximum contaminant radius. Thus, the recommended value of this parameter is 101. It may be desirable for users to determine the effect of varying the size of the source on the aquifer concentrations.

Minimum output concentration (mg/L)

Enter the minimum concentration (mg/L) for TSGPLUME to include in the output. Concentrations below this value will be reported as zero. A nonzero value of this parameter is required for proper execution of the TSGPLUME module. Typically, a concentration of 0.001 mg/L is suitable for the minimum concentration.

Beginning time (d)

Enter the beginning time in days for the TSGPLUME simulation. See note below.

Ending time (d)

Enter the ending time in days for the TSGPLUME simulation. See note below.

Time increment (d)

Enter the time increment in days for TSGPLUME output between the beginning and ending times specified above. Typically 50 or 100 days is adequate for the time increment.

NOTE: Before running the model, it is not possible to guess precisely when the contaminant arrives at or passes a given receptor point. HSSM-T will override the user supplied beginning and ending times which allows the model to produce smooth concentration histories at the receptor point. Particular effort is expended in HSSM-T to calculate when the contaminant first arrives at the receptor point and when the peak concentration arrives. The duration of mass flux into the aquifer is used to determine a proposed time increment for HSSM-T output. If one hundredth of the mass flux input duration is greater than the user specified time increment the user is prompted to increase the time increment:

```
*** TSGPLUME RECOMMENDS CHANGING THE TIME INCREMENT
*** FROM  0.5000 DAYS TO 98.60 DAYS
*** ACCEPT THE CHANGE ? (Y OR N)
```

HSSM-T is making the user an offer that shouldn't be refused, at least for an initial simulation. If the resulting concentration history curve is not smooth enough, the user may reduce the time increment for HSSM-T to produce a finer spacing in time.

If the user does not accept the change, he/she is prompted to decide between the original time increment or to enter a new time increment.

NAPL LENS PROFILES

Number of profiles

Enter the number of KOPT saturation vs depth profiles (**Saturation Profiles** graph) and OILENS lens thickness vs. radius profiles (**NAPL Lens Profiles** graph). Both are produced at the specified times along with mass balance approximations. Up to ten profiles are allowed.

Time of profiles

Enter up to ten profile times in days. The number of entries will be automatically truncated to match the value of **Number of profiles** above.

RECEPTOR LOCATIONS

These values are used by the TSGPLUME model only.

Number of wells

Enter the number of wells (a maximum of six) for which TSGPLUME is to calculate concentration vs time for the **Well Concentrations** graph.

Locations of wells

Enter up to six well locations, as X and Y coordinates in meters. X is the directed along the longitudinal axis of the plume (the direction of groundwater flow) and Y is directed transversely to the X axis. The origin of the coordinate system is located at the center of the source (see **Figure 9**). The number of entries will be truncated depending on the value of **Number of wells** above.

4.7 Running the KOPT, OILENS and TSGPLUME Modules

This section describes the operation of the HSSM-KO and HSSM-T modules. These programs are the heart of the simulation model. Both of the modules are DOS programs which are executed by selecting HSSM-WIN menu items. Once an input data file has been created the HSSM-KO module is executed by selecting the "Run HSSM-KO" menu item *(3a* on Table 7*)* Table 12 shows the first screen that appears when HSSM-KO is executed. This screen identifies the model and the authors. Pressing return displays the disclaimer screen (Table 13) . Carefully note the disclaimer messages. Sound scientific and engineering judgement is required when applying models and the user is responsible for the application of the model.

Table 12 Introductory HSSM-KO Screen

```
***************************************************
*                                                 *
*                    HSSM                         *
*                                                 *
*        HYDROCARBON SPILL SCREENING MODEL        *
*                                                 *
*  INCLUDING THE KOPT, OILENS AND TSGPLUME MODELS *
*                                                 *
*               JAMES W. WEAVER                   *
*  UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  *
*   R.S. KERR ENVIRONMENTAL RESEARCH LABORATORY   *
*             ADA, OKLAHOMA 74820                 *
*                                                 *
*  INCLUDING OILENS--HYDROCARBON MOVEMENT ON THE  *
*                 WATER TABLE                     *
*  RANDALL CHARBENEAU, SUSAN SHULTZ, MIKE JOHNSON *
*   ENVIRONMENTAL AND WATER RESOURCES ENGINEERING *
*       THE UNIVERSITY OF TEXAS AT AUSTIN         *
*                                                 *
*                 VERSION 1.00                    *
***************************************************
```

Table 13 Disclaimer Screen

```
***************************************************
 *                     WARNING:                    *
 * THIS PROGRAM SIMULATES IDEALIZED BEHAVIOR OF    *
 * OILY-PHASE CONTAMINANTS IN IDEALIZED POROUS     *
 * MEDIA, AND IS NOT INTENDED FOR APPLICATION TO   *
 * HETEROGENEOUS SITES.                            *
 * THE MODEL RESULTS HAVE NOT BEEN VERIFIED BY     *
 * EITHER LAB OR FIELD STUDIES.                    *
 * READ USER GUIDE FOR FURTHER INFORMATION BEFORE  *
 * ATTEMPTING TO USE THIS PROGRAM.                 *
 * NEITHER THE AUTHORS, THE UNIVERSITY OF TEXAS,   *
 * NOR THE UNITED STATES GOVERNMENT ACCEPTS ANY    *
```

A list of the file names used by HSSM-KO and HSSM-T is displayed in Table 14.

Table 14 Output File Names and Run Options

```
OUTPUT AND PLOT FILE NAMES:

HSSM-KO INPUT DATA FILE    BENZENE.DAT
HSSM-KO OUTPUT             BENZENE.HSS
HSSM-KO PLOT 1             BENZENE.PL1
HSSM-KO PLOT 2             BENZENE.PL2
HSSM-KO PLOT 3             BENZENE.PL3
HSSM-T INPUT DATA FILE     BENZENE.PMI
HSSM-T OUTPUT              BENZENE.TSG
HSSM-T PLOT                BENZENE.PMP

TO RUN HSSM-KO          ENTER <RETURN>
TO EXIT                 ENTER 1
```

The names must follow a strict naming convention for the TSGPLUME module (HSSM-T) and the post-processors to function properly. Table 15 gives the required file names. For the user's convenience the correct file names are generated automatically by either of the interfaces. These should not be modified by the user.

As summarized in Table 15, there are eight files associated with each simulation, all with the same prefix (eight characters or fewer) but different extensions (three characters). ***.DAT** identifies a *data file*, which is edited by HSSM-WIN or PRE-HSSM and read by the HSSM-KO program as an input file. The HSSM-KO module generates up to five other files: ***.HSS**, ***.PL1**, ***.PL2**, ***.PL3** and ***.PMI**. The *plot files*, ***.PL1**, ***.PL2**, and ***.PL3** contain data which HSSM-WIN or HSSM-PLT uses to generate graphs, and the output file, ***.HSS**, contains neatly formatted and labelled data for reference. HSSM-KO optionally produces the ***.PMI** file, an input file for the HSSM-T program. HSSM-T itself produces two similar files: ***.PMP** (a plot file), and ***.TSG** (a formatted text file).

Table 15 Files Used by the HSSM interfaces

Extension	Created by	Used by	Purpose
.DAT	HSSM-WIN or PRE-HSSM	HSSM-KO	data input
.PMI	HSSM-KO	HSSM-T	data input
.HSS	HSSM-KO	the user	text output
.TSG	HSSM-T	the user	text output
.PL1	HSSM-KO	HSSM-WIN or HSSM-PLT	data for plotting
.PL2	HSSM-KO	HSSM-WIN or HSSM-PLT	data for plotting
.PL3	HSSM-KO	HSSM-WIN or HSSM-PLT	data for plotting
.PMP	HSSM-T	HSSM-WIN or HSSM-PLT	data for plotting

As indicated in Table 14 the user may either run HSSM-KO or exit the program. Upon beginning a simulation the model writes messages to the screen as the computations proceed. These allow the simulation to be tracked by the user. Table 16 contains a typical set of screen messages for a simulation.

Table 16 Typical HSSM-KO Screen Messages

```
*** DATA INPUT
*** DATA INITIALIZATION
*** SIMULATION BEGINNING
*** OIL INFILTRATION
*** OIL REDISTRIBUTION
*** CHEMICAL REACHES WATER TABLE
*** OIL LENS FORMS
*** PROFILING AT      15.00 DAYS
*** PROFILING AT      30.00 DAYS
*** PROFILING AT      90.00 DAYS
*** PROFILING AT     130.00 DAYS
*** PROFILING AT     175.00 DAYS
*** SIMULATION END
*** POST PROCESSING
*** CREATING OUTPUT FILE:
*** BENZENE.HSS
*** PROCESSING PLOT FILE CONTENTS
*** REPACKING FILE 18
*** REPACKING FILE 19
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL1
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL2
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL3
*** CREATING TSGPLUME DATA FILE:
*** BENZENE.PMI
*** HSSM END
```

Upon completing the HSSM-KO simulation, the DOS window remains open so that any error messages stay on the screen. The window is closed by clicking on its system menu (upper left hand corner) and selecting exit.

The HSSM-T implementation of TSGPLUME is designed to be used with HSSM-KO. If the data set for HSSM-KO has switches set appropriately, and if the dissolved chemical of interest reaches the water table (either through the formation of a NAPL lens or by the leaching from an immobilized NAPL body in the vadose zone), then an input data set for TSGPLUME is created by running HSSM-KO. The necessary flags and conditions for TSGPLUME data file generation are summarized in Table 17. These parameters are described in detail in the Section 4.6.6.

Table 17 HSSM-KO Data Switches for the Creation of TSGPLUME (HSSM-T) input Data Files

Condition or switch	Dialog box	Effect
☒ Create output files	General	Output and plot files produced
☒ Run KOPT	General	KOPT module is run
☒ Run OILENS	General	OILENS module is run
☒ Dissolved constituent exists	Hydrocarbon Phase	Chemical constituent is included in the simulation.
☒ Write HSSM-T input file	General	Attempt to create the TSGPLUME (HSSM-T.EXE) input data.
OILENS Simulation ending criterion ◉ Contaminant leached from lens	Simulation Parameters	End HSSM-KO.EXE simulation when a small fraction of chemical constituent remains in the oil lens.
"large" Simulation ending time	Simulation Parameters	Allow sufficient simulation time for chemical to reach the water table before ending simulation.

Once HSSM-KO has run and produced an HSSM-T input data file, HSSM-T can be executed by selecting the Run HSSM-T menu item *(3b* on Table 7*)*. When HSSM-T executes, screen messages appear as shown in Table 18. After pressing return, the file names for the simulation appear as indicated in Table 19.

Table 18 Introductory HSSM-T Screen

```
***************************************************
*                                                 *
*                   TSGPLUME                      *
*                                                 *
*      TRANSIENT SOURCE GAUSSIAN PLUME MODEL      *
*                                                 *
*                                                 *
*                  MIKE JOHNSON                   *
*               RANDALL CHARBENEAU                *
*        THE UNIVERSITY OF TEXAS AT AUSTIN        *
*                                                 *
*                   JIM WEAVER                    *
* ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY*
*  UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  *
*                                                 *
*                 VERSION 1.00                    *
***************************************************
```

Table 19 HSSM-T Output File Names and Run Options

```
OUTPUT AND PLOT FILE NAMES:

HSSM-KO INPUT DATA FILE  BENZENE.DAT
HSSM-KO OUTPUT           BENZENE.HSS
HSSM-T INPUT             BENZENE.PMI
HSSM-T OUTPUT            BENZENE.TSG
HSSM-T PLOT              BENZENE.PMP

TO RUN TSGPLUME          ENTER <RETURN>
TO EXIT                  ENTER 1
```

When HSSM-T executes, a set of messages is written to the screen (Table 20). These messages inform the user on the progress of the simulation. The example shown has only one receptor location; when more receptors are used, more messages like these are produced.

Table 20 Typical HSSM-T Screen Messages

```
  *** DATA INPUT
  *** DATA INITIALIZATION
  *** CALCULATING FLOATING POINT PRECISION
  ***
  *** COMPUTATION BEGINNING FOR RECEPTOR     1
  *** CALCULATING THE TOE TIME OF THE HISTORY
  *** SEARCH ALGORITHM COMPLETED IN    6 ITERATIONS
  *** COMPUTATION AT  18.18     DAYS COMPLETED
  *** COMPUTATION AT  18.44     DAYS COMPLETED
  *** COMPUTATION AT  33.41     DAYS COMPLETED
  *** COMPUTATION AT  48.38     DAYS COMPLETED
  *** COMPUTATION AT  63.35     DAYS COMPLETED
  *** COMPUTATION AT  78.32     DAYS COMPLETED
  *** COMPUTATION AT  83.32     DAYS COMPLETED
  *** COMPUTATION AT  88.32     DAYS COMPLETED
  *** COMPUTATION AT  93.32     DAYS COMPLETED
  *** COMPUTATION AT  98.32     DAYS COMPLETED
  *** COMPUTATION AT  103.3     DAYS COMPLETED
  *** COMPUTATION AT  108.3     DAYS COMPLETED

{other similar messages omitted}

  *** COMPUTATION AT  553.3     DAYS COMPLETED
  *** COMPUTATION AT  603.3     DAYS COMPLETED
  *** COMPUTATION AT  653.3     DAYS COMPLETED
  *** COMPUTATION AT  703.3     DAYS COMPLETED
  *** COMPUTATION AT  753.3     DAYS COMPLETED
  *** COMPUTATION AT  803.3     DAYS COMPLETED
  *** COMPUTATION AT  853.3     DAYS COMPLETED
  ***
  *** OUTPUT FILE:
  ***    BENZENE1.TSG
  *** PLOT FILE:
  ***    BENZENE1.PMP
  *** TSGPLUME END
```

Upon completing the HSSM-T simulation, the DOS window remains open so that any error messages stay on the screen. The window is closed by clicking on its system menu (upper left hand corner) and selecting exit.

4.8 Graphical Presentation of HSSM Output

Six graphs can be automatically generated from a successful HSSM simulation. These graphs provide a visual summary of the simulation results and include information from each of the three modules of HSSM. Table 21 gives information on each of the graphs provided.

Table 21 HSSM Graphics

Title	HSSM Module	Description
Saturation Profiles	KOPT	Vadose Zone Liquid Saturations from the Surface to the Water Table
NAPL Lens Profiles	OILENS	Cross-section of the NAPL lens on the water table
NAPL Lens Radius History	OILENS	History of the radius of the NAPL lens and the effective radius of the contaminant
Contaminant Mass Flux History	OILENS	History of the mass flux from the NAPL lens to the aquifer
NAPL Lens Contaminant Mass Balance	OILENS	History of the mass in the NAPL lens
Receptor Concentration Histories	TSGPLUME	History of the contaminant concentrations at the receptor points

Each of the graphics is described in the following sections along with an example figure.

4.8.1 Saturation Profiles

The saturation profiles (**Figure 23**) represent the simulated distribution of fluids in the vadose zone. The cross-hatched region on the left represents the assumed uniform water saturation. Plotted between the water saturation and "1.0" are the NAPL profiles. The profiles are created at the profile times selected by the user before running the model. The profile times are listed on the lower right of the figure. The times correspond to the profiles plotted from right to left (i.e., the outermost profile corresponds to the earliest time). The profiles may not turn out to be plotted at advantageous times for display of the results. The user may wish to rerun the model with modified times in order to produce a desired sequence of profiles.

4.8.2 NAPL Lens Profiles

The lens profile graph (**Figure 24**) illustrates the configuration of the lens at the profile times selected by the user. The graph illustrates the configuration of the lens in the vicinity of the water table (vertical axis). The water table is indicated by the horizontal line. The horizontal axis shows the lens radius beginning at the source (radius = 0.0) out to some distance beyond the edge of the lens. The vertical line from the top to the lens indicates contamination in the vadose zone due to the source. The saturation profiles give the time variation of saturation within this region. The lens shaped body shows the configuration of the actively spreading NAPL. The hatched areas (which are barely visible in this example) indicate the region of the vadose and saturated zones where there is residual NAPL. These regions develop as the NAPL lens builds and then decays. To step through the sequence of lens profiles, click on the arrow buttons at the upper left of the graph.

4.8.3 Contaminant Mass Flux History

The contaminant mass flux history (**Figure 25**) shows the mass flux of contaminant into the aquifer as a function of time. This mass flux is used as the input boundary condition to HSSM-T. As the NAPL lens forms, the mass flux to the aquifer increases rapidly, due to the increasing radius of the NAPL lens. If the source is cut off, as occurs in this example, the mass flux to the aquifer declines because of leaching of the contaminant into the aquifer. Typically, the mass flux shows a "tailing" effect. In fact, if this graph does not show decline of the mass flux into the aquifer, then the input mass flux to HSSM-T has been truncated and the HSSM-T results are likely in error.

4.8.4 NAPL Radius History

The NAPL lens radius history shows the radius of the lens as a function of time (**Figure 26**). The lens radius increases rapidly as the gasoline enters the lens. Later the lens tends toward a limiting radius.

4.8.5 NAPL Lens Contaminant Mass Balance

The NAPL lens contaminant mass balance (**Figure 27**) shows the mass of contaminant contained within the NAPL lens as a function of time. The graph also plots the cumulative mass of contaminant which has been dissolved into the ground water from the lens. As the mass contained within the lens declines, the cumulative mass dissolved increases proportionately.

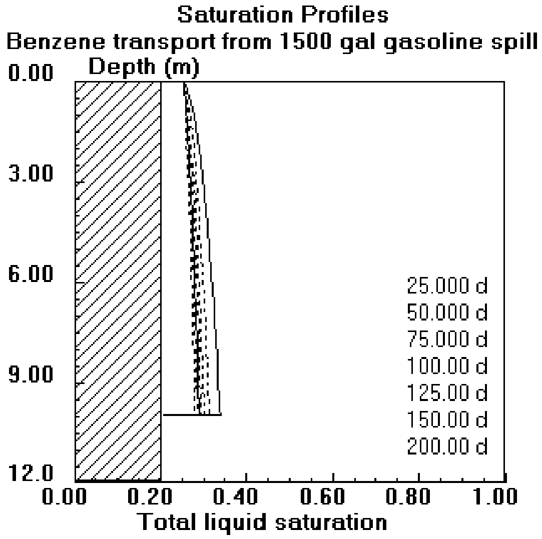


Figure 23 Typical saturation profiles

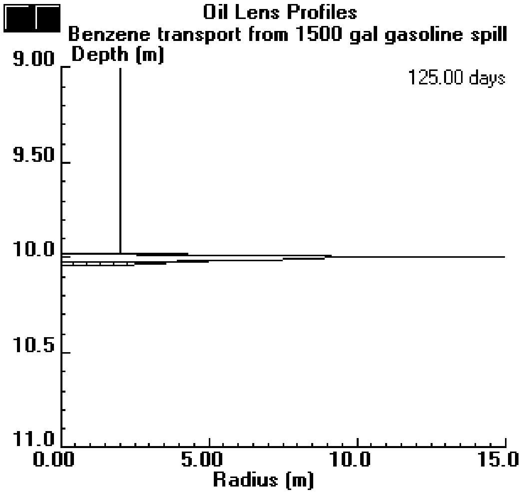


Figure 24 Typical NAPL lens profile

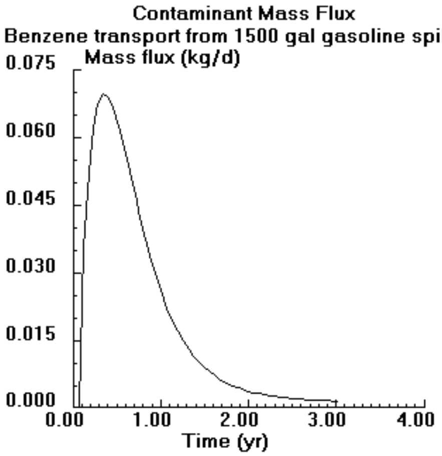


Figure 25 Typical contaminant mass flux history

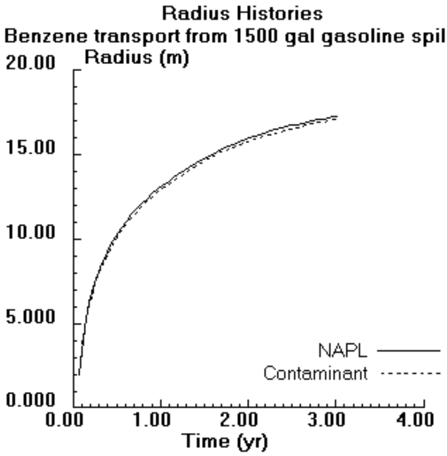


Figure 26 Typical NAPL lens radius history

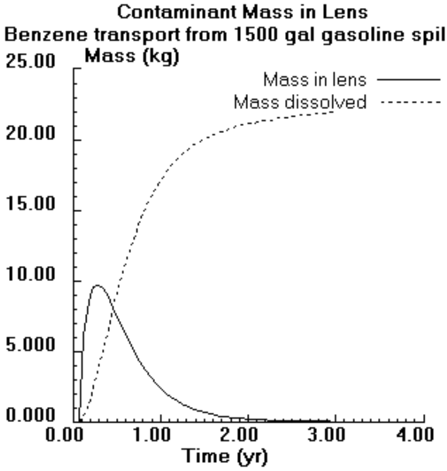


Figure 27 Typical NAPL lens contaminant mass balance

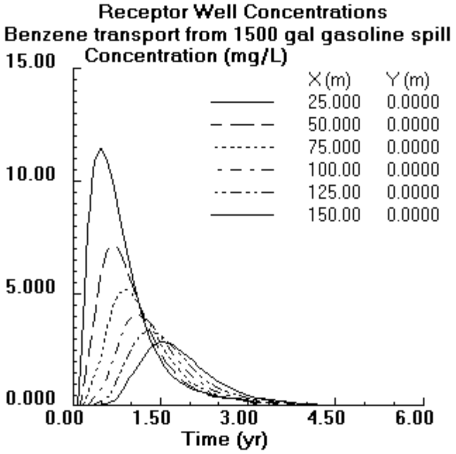


Figure 28 Typical receptor concentration histories

4.8.6 Receptor Concentration Histories

The receptor concentration histories (**Figure 28**) show the predicted concentrations at the user-selected receptor points. Concentrations above the specified threshold are plotted as a function of time for each receptor location. Care should be taken to identify the threshold value input to the model in order to assure that the value has not been set too high and as a result truncated concentration histories are plotted in this graph.

4.9 A Note on the Efficiency of Using the Windows Interface

The computational modules of HSSM (HSSM-KO and HSSM-T) execute more rapidly under DOS than they do under Windows. Within Windows, the HSSM-KO and HSSM-T models run faster as a full screen process than in a DOS window. In some cases, the most time-efficient way to use the Windows interface is to use HSSM-WIN as a preprocessor to create several input data files, then exit HSSM-WIN and run HSSM-KO and HSSM-T under DOS (Appendix 1.9). The commands for running HSSM-KO and HSSM-T from DOS are

```
HSSM-KO name.dat
HSSM-T name.pmi
```

where **name.dat** is the input data set created by HSSM-WIN and name.pmi is the HSSM-T input data file created by running HSSM-KO. The results can be viewed by reentering HSSM-WIN and plotting graphs of the results.

4.10 Menu Command Reference

This section lists each HSSM-WIN command an briefly describes its action. The italicized number and letter refer to the columns and rows of Table 7, respectively.

File *(1)*

The File menu lists commands for manipulating files, and includes the option to Exit HSSM-WIN.

New *(1.a)*
New clears the memory of parameters and file names, restoring HSSM-WIN to its startup state.

Open... *(1.b)*
The Open dialog box (**Figure 13**) is used to open a data file. This file contains the input data for the model programs. Once opened by HSSM-WIN, the data are available for editing or saving under a new name.

Save *(1.c)*
Save will save the current parameter settings in the current file, which is displayed in HSSM-WIN's caption bar.

Save As... *(1.d)*
The Save As dialog box (**Figure 14**) will prompt for an alternate file name under which to save the current settings. When entering the name, it is sufficient to enter only the prefix (the first eight or fewer characters). HSSM-WIN will tack on the appropriate extension if you have not.

Check File Times *(1.e)*

This selection checks the file creation or modification times to prevent HSSM-T from being executed with an outdated input file. Normally, if an HSSM-KO input data file has been modified, HSSM-T should not be run before HSSM-KO has been run or rerun.

When this selection is activated, HSSM-T is prevented from being executed if the HSSM-KO input data file has a later date/time than the HSSM-T input data file. Plotting files are also checked to see if they predate the data input files, in which case the user is prompted to rerun the model. Sometimes, as when files are moved from one directory to another, the user may wish to override this safety feature.

Exit HSSM-WIN *(1.f)*
This selection is used to terminate HSSM-WIN and clear the screen of all graphs.

Edit *(2)*

General Data *(2.a)* is used to set various model switches and to select titles for the graphs.

Hydrologic Data *(2.b)* is used to input hydrologic and hydraulic variables.

Hydrocarbon Phase Data *(2.c)* is used to choose parameters related to the NAPL phase and the chemical constituent.

Model Simulation Data *(2.d)* is used to input options which control the simulations by HSSM-KO and HSSM-T.

Information about the meaning and appropriate values for each item in the data entry dialog boxes is given in Sections 4.6.3 through 4.6.6.

Model *(3)*

Run HSSM-KO *(3.a)*
Causes HSSM-KO to execute under using the current HSSM-KO input data file.

Run HSSM-T *(3.b)*
Causes HSSM-T to execute using the current HSSM-T input data file.

Run REBUILD *(3.c)*
Causes REBUILD to execute and attempt to recover temporary files from an interrupted or unsuccessful run.

Graph *(4)*

The **Display Graphs** *(4.a)* dialog box (**Figure 15**) will prompt the user for which graphs to generate and will draw them on the screen.

In the event that no oil lens has formed or the TSGPLUME model was not run, some graphs will not be available for display, and their checkboxes will be empty. Attempting to select these boxes will produce a message about their unavailability. For example, in **Figure 15** the Receptor Well Concentrations are not available.

Copy Graph *(4.b)* copies the contents of the graph window, in its current size and configuration, to the Windows Clipboard, a data storage facility available to all Windows applications. Once copied to the Clipboard, the graph can be transferred to other applications such as PAINTBRUSH or WRITE using the "Paste" command within those applications. Nothing can be pasted into HSSM-WIN, but the graphs can be exported as bitmaps this way.

Print Graph *(4.d)* prints a copy of the graph on the printer that Windows currently recognizes. (Choice of printers is available through the Windows Control Panel). HSSM-WIN attempts to make an actual size copy of the graph window on the printed page, so what appears in the graph window is what will appear on paper. Small graphs print fairly quickly (several seconds), but larger ones will take longer since there are more points to transfer. A full-screen graph will be scaled down to fit on the page, and may take several minutes, depending on the sophistication of the printer.

HSSM-WIN's print function does not support plotters or daisy-wheel printers, since they cannot print bitmaps.

Close Graph *(4.e)* closes the currently selected graph. Graphs may also be closed by double clicking on their system menus.

Fonts *(4.f)* allows the selection of alternative fonts for lettering the HSSM graphics. Various fonts may be chosen for the graph title, axis labels, and legends. The **default** option returns all graph text to the default font.

Window *(5)*

Cascade *(5.a)*
Arranges the graph windows in a cascaded formation.

Tile *(5.b)*
Arranges the graph windows in a tiled formation.

Arrange Icons *(5.c)*
Neatly rearranges the graph icons. The spacing of these icons is determined by the setting in the Desktop applet in control panel.

Close All *(5.d)*
Closes all of the graph windows and removes them from memory.

Help *(6)*

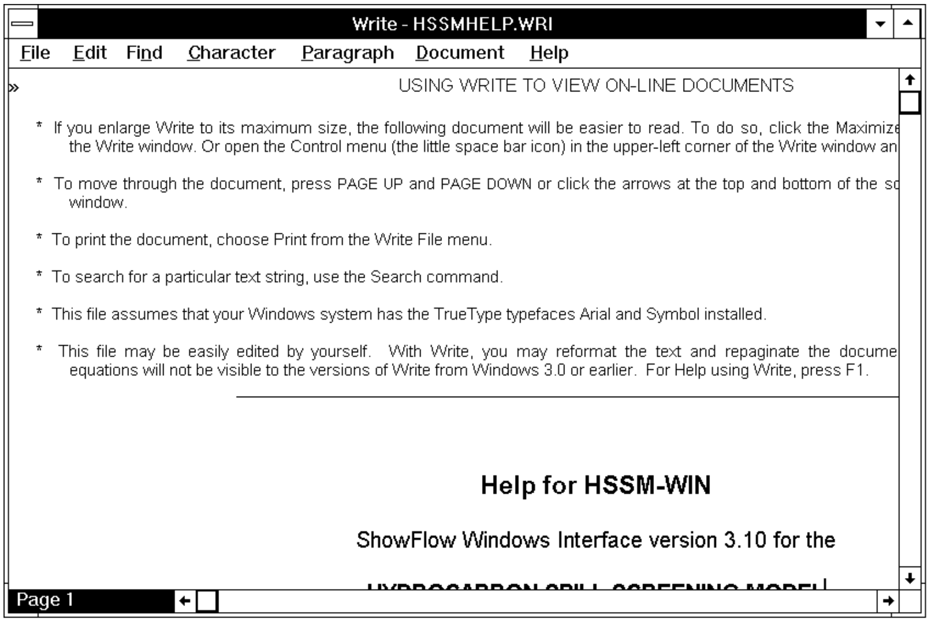
Read Help File *(6.a)*
The Help file, HSSMHELP.WRI, can be read using WRITE, the standard file editor which comes bundled with Windows. **Figure 29** shows a sample of this Help file.

About HSSM and **About HSSM-WIN** *(6.b* and *6.c)*

The "About" dialog boxes provide information pertaining to the origins of the programs.

The System Menu *(7)*

The system menu, common to all windows programs, is accessed by clicking on the spacebar icon in the upper left corner of the window or by typing ALT + SPACEBAR from the keyboard. In addition to choosing various modes of display of the window, the program may also be terminated.



USING WRITE TO VIEW ON-LINE DOCUMENTS

- If you enlarge Write to its maximum size, the following document will be easier to read. To do so, click the Maximize
  the Write window. Or open the Control menu (the little space bar icon) in the upper-left corner of the Write window an
- To move through the document, press PAGE UP and PAGE DOWN or click the arrows at the top and bottom of the sc
  window.
- To print the document, choose Print from the Write File menu.
- To search for a particular text string, use the Search command.
- This file assumes that your Windows system has the TrueType typefaces Arial and Symbol installed.
- This file may be easily edited by yourself. With Write, you may reformat the text and repaginate the docume
  equations will not be visible to the versions of Write from Windows 3.0 or earlier. For Help using Write, press F1.

Help for HSSM-WIN

ShowFlow Windows Interface version 3.10 for the

HYDROCARBON SPILL SCREENING MODEL

Figure 29 HSSM-WIN "Help" information in HSSMHELP.TXT

Section 5 Example Problems

In this section, two example problems are presented along with HSSM input data sets and graphic of the results. The complete set of input and output files is distributed on the HSSM-2 diskette. The intent of these examples is to provide guidance in application of the model to similar problems. Each begins with a brief description of the problem including some values of model parameters which are assumed to be well-known. The examples then proceed with a discussion of the specific rationale used for the selection of each parameter of the model. The parameters are listed in the order that they appear in the Windows interface.

5.1 Problem 1: Gasoline Arrival Time at the Water Table

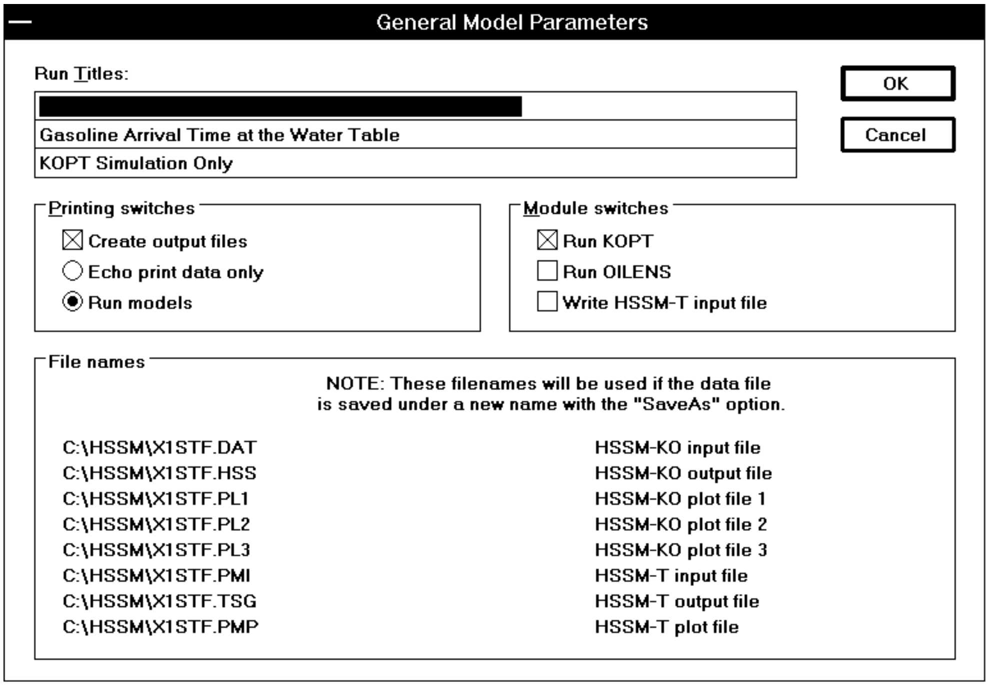
An emergency response and monitoring plan is being prepared for an above-ground storage tank facility. An estimate is needed of how long it would take gasoline to reach the water table and what monitoring frequency would be required to detect a leak before gasoline reaches the water table. The soil has been classified as a sandy clay loam soil. In this example, the water table lies at a depth of 5.0 meters. All of the parameters for the model run are saved in the file **X1STF.DAT**. HSSM-WIN can be used to page through the input parameters as the example is studied. The file may be loaded and viewed according to the instructions in section 4.5.2 "Creating and Editing Input Data Sets."

This problem needs the use of the KOPT module with no dissolved contaminant. A "per unit area" simulation should be performed because only the transport time through the vadose zone is required. Of all the input data required for the model, only the following parameters are required for the "KOPT only" simulation. HSSM-WIN places necessary zeros in the data file for the unused parameters. The presentation of the input data follows the order of the four HSSM-WIN input data dialog boxes.

The first of the boxes, "General Model Parameters," contains the run title, printing switches, module switches and the file names. For this example, the run title is

Gasoline Release from an Aboveground Storage Tank Fac.
Gasoline Arrival Time at the Water Table
KOPT Simulation Only

The "create output files" switch is checked in order to write the output files. For the first attempt at running a new data set, it is recommended to echo print the input data only and check the parameter values by reading the ***.HSS** output file. Only the Run KOPT module switch is checked as only KOPT is needed to estimate the gasoline arrival time at the water table. The output file names are automatically generated by the interface and shown in the FILE names area of the dialog box. The file name used for this simulation is **X1STF.DAT**. The completed dialog box appears as shown in **Figure 30**.



Run Titles:

[redacted]

Gasoline Arrival Time at the Water Table

KOPT Simulation Only

Printing switches

☒ Create output files
○ Echo print data only
● Run models

Module switches

☒ Run KOPT
☐ Run OILENS
☐ Write HSSM-T input file

File names

NOTE: These filenames will be used if the data file
is saved under a new name with the "SaveAs" option.

C:\HSSM\X1STF.DAT	HSSM-KO input file
C:\HSSM\X1STF.HSS	HSSM-KO output file
C:\HSSM\X1STF.PL1	HSSM-KO plot file 1
C:\HSSM\X1STF.PL2	HSSM-KO plot file 2
C:\HSSM\X1STF.PL3	HSSM-KO plot file 3
C:\HSSM\X1STF.PMI	HSSM-T input file
C:\HSSM\X1STF.TSG	HSSM-T output file
C:\HSSM\X1STF.PMP	HSSM-T plot file

Figure 30 Problem 1 completed General Parameters dialog box

The second dialog box, "Hydrologic Parameters" contains the hydrologic and soil properties.

Hydrologic Properties

The parameters shown in Table 22 are used for the Hydrologic Properties. Standard fluid properties are used for the water phase. During infiltration, some of the air in the pore space is not displaced by either the water or the NAPL. It is assumed that during infiltration the maximum hydraulic conductivity to water is one-half of the saturated hydraulic conductivity. From this assumption, HSSM automatically determines the amount of air trapped in the pore space.

Table 22 Problem 1 Hydrologic Properties

Parameter	Rationale	Value
Water Phase Viscosity, μ_w	Standard value	1.0 cp
Water Phase Density, ρ_w	Standard value	1.0 g/cm^3
Water Phase Surface Tension, σ_{aw}	Assumed	65.0 dyne/cm
Maximum Relative Permeability During Infiltration, $k_{rw(max)}$	Assumed	0.5
Recharge Input Type	Specify Saturation	
Water Saturation, $S_{w(max)}$	Specified water saturation	0.35

Capillary Pressure Curve Model and Porous Medium Properties

The porous medium properties are estimated from Brakensiek et al.'s soil parameter tabulation for the Brooks and Corey model. The values shown in Table 23 are taken from the tabulation reproduced in Appendix 3.1.

Table 23 Problem 1 Porous Medium Properties

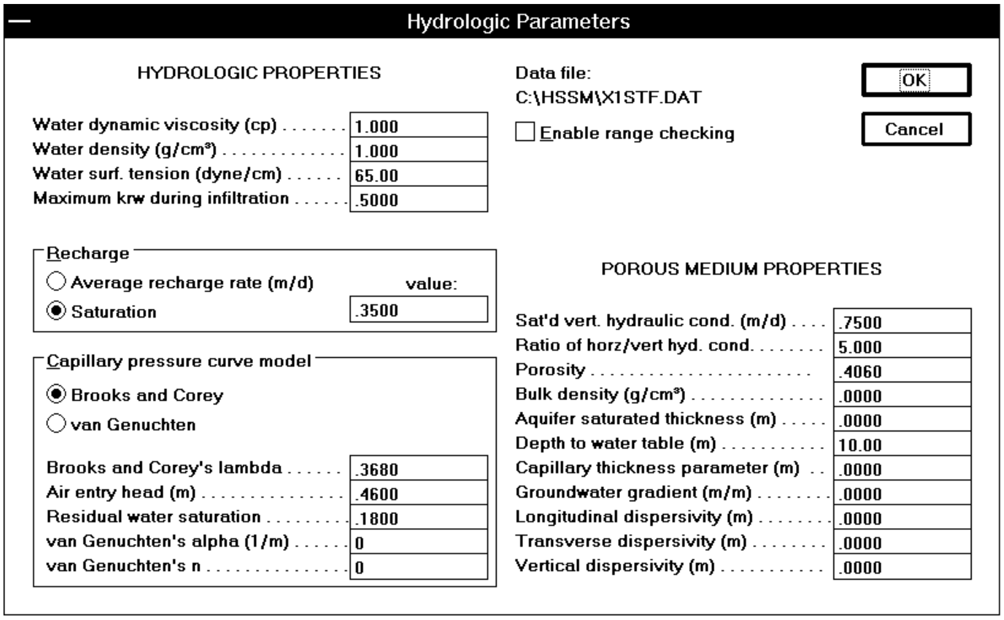
Parameter	Value
Brooks and Corey's Pore Size Distribution Index, λ	0.368
Air Entry Head, h_{ce}	46.3 cm
Residual Water Content, θ_{wr}	0.075
Porosity, η	0.406

The residual water saturation that is required by HSSM is calculated by dividing the residual water content by the porosity to get 0.18 (0.075/0.406).

The hydraulic conductivity in cm/s of the system is then estimated from (Brakensiek et al., 1981)

$$K_s = 270 \frac{\eta^2}{h_{ce}^2} \frac{\lambda^2}{(\lambda + 1)(\lambda + 2)} = 8.68 \, x \, 10^{-4} \, cm/s \tag{17}$$

where the air entry head is in centimeters. The value is then converted to the units of meters per day by multiplying by 864 to give a K_s of 0.75 m/d. From the basic soil property information, the following parameters are determined (Table 24). The completed dialog box is shown in **Figure 31**. Note that in all of the dialog boxes for Problem 1 range checking is disabled. This is shown by the open check box (☐) below the file name. Range checking must be disabled for KOPT only simulations, because many of the input parameters default to normally-disallowed zeros.



HYDROLOGIC PROPERTIES

Water dynamic viscosity (cp) 1.000
Water density (g/cm³) 1.000
Water surf. tension (dyne/cm) 65.00
Maximum krw during infiltration ...... .5000

Recharge
○ Average recharge rate (m/d) value:
● Saturation .3500

Capillary pressure curve model
● Brooks and Corey
○ van Genuchten

Brooks and Corey's lambda ...... .3680
Air entry head (m) .... .4600
Residual water saturation .... .1800
van Genuchten's alpha (1/m) 0
van Genuchten's n 0

Data file:
C:\HSSM\X1STF.DAT
☐ Enable range checking

POROUS MEDIUM PROPERTIES

Sat'd vert. hydraulic cond. (m/d) .... .7500
Ratio of horz/vert hyd. cond. 5.000
Porosity .... .4060
Bulk density (g/cm³) .... .0000
Aquifer saturated thickness (m) ..... .0000
Depth to water table (m) 10.00
Capillary thickness parameter (m) .. .0000
Groundwater gradient (m/m) .... .0000
Longitudinal dispersivity (m) .... .0000
Transverse dispersivity (m) .... .0000
Vertical dispersivity (m) .... .0000

Figure 31 Problem 1 completed Hydrologic Properties dialog box

Table 24 Problem 1 Hydraulic Conductivity and Capillary Pressure Curve Parameters

Parameter	**Rationale**	**Value**
Ratio of Horizontal to Vertical Conductivity	Arbitrary value as this parameter is not used in KOPT	5.0
Porosity, η	From Brakensiek et al. 1981 Tabulation	0.406
Depth to Water Table	Arbitrary value as only KOPT is used	10.0 m

Hydrocarbon Phase Parameters

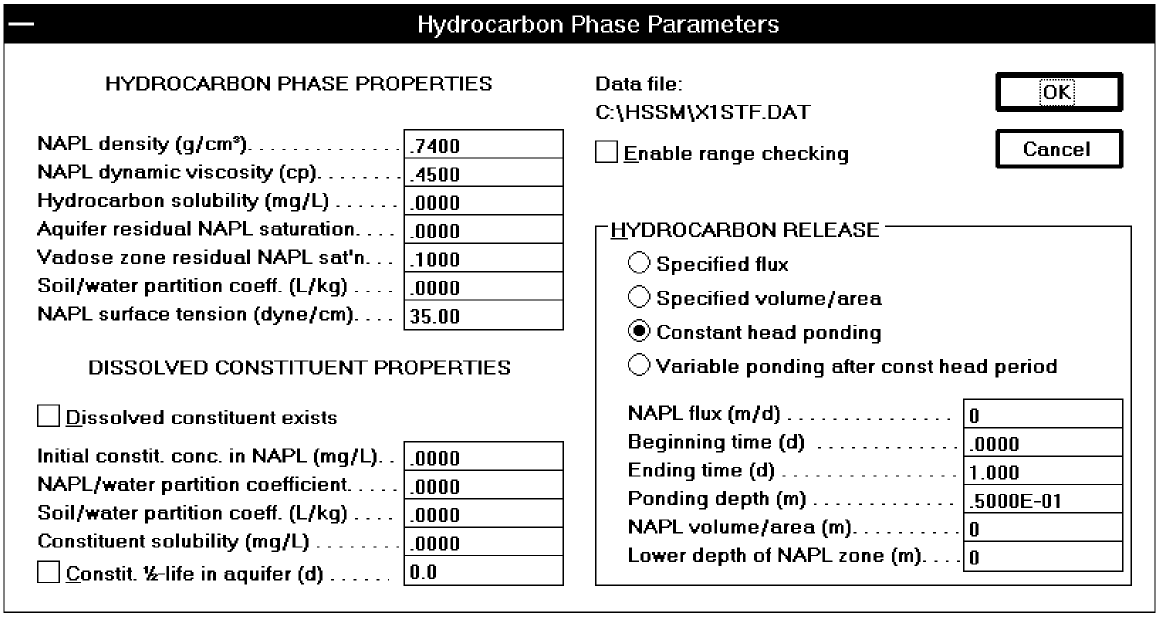
Table 25 shows the NAPL fluid property values that are entered in **Figure 32**. These are intended to represent gasoline.

Table 25 Problem 1 Hydrocarbon (NAPL) Phase Properties

Parameter	Rationale	Value
NAPL Phase Density, ρ_o	Typical value for gasoline	0.74 g/cm^3
NAPL Phase Viscosity, μ_o	Typical value for gasoline	0.45 cp
Residual NAPL Saturation (vadose zone), S_{orv}	Estimated	0.10
NAPL Surface Tension, σ_{ao}	Estimated	35.0 dyne/cm

Hydrocarbon Release

The hydrocarbon (NAPL) release scenario is chosen by selecting the radio button for constant head ponding (**Figure 32**). The beginning time, ending time and ponding depth are entered to define the release. The release is assumed to begin at 0.0 days and end at 1.0 day. During this interval the ponding depth is assumed to remain constant at 0.05 m (5 cm).



HYDROCARBON PHASE PROPERTIES

NAPL density (g/cm³)	.7400
NAPL dynamic viscosity (cp)	.4500
Hydrocarbon solubility (mg/L)	.0000
Aquifer residual NAPL saturation	.0000
Vadose zone residual NAPL sat'n.	.1000
Soil/water partition coeff. (L/kg)	.0000
NAPL surface tension (dyne/cm)	35.00

DISSOLVED CONSTITUENT PROPERTIES

☐ Dissolved constituent exists

Initial constit. conc. in NAPL (mg/L)	.0000
NAPL/water partition coefficient	.0000
Soil/water partition coeff. (L/kg)	.0000
Constituent solubility (mg/L)	.0000
☐ Constit. ½-life in aquifer (d)	0.0

Data file:
C:\HSSM\X1STF.DAT

☐ Enable range checking

HYDROCARBON RELEASE

○ Specified flux
○ Specified volume/area
● Constant head ponding
○ Variable ponding after const head period

NAPL flux (m/d)	0
Beginning time (d)	.0000
Ending time (d)	1.000
Ponding depth (m)	.5000E-01
NAPL volume/area (m)	0
Lower depth of NAPL zone (m)	0

Figure 32 Problem 1 completed Hydrocarbon Phase Properties dialog box

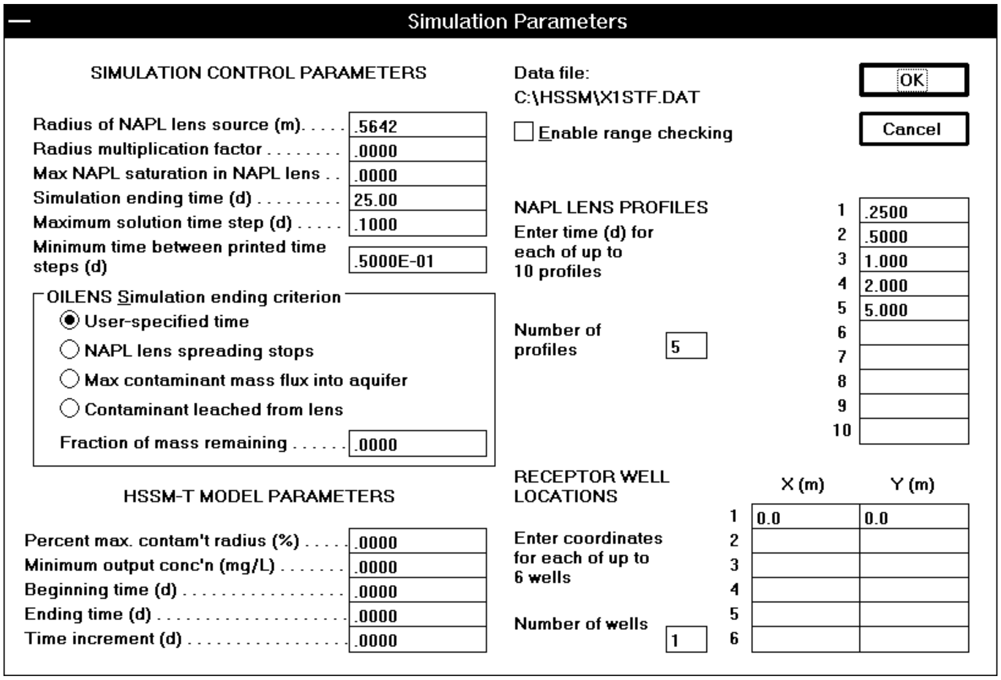
Simulation Parameters

The remaining parameters are shown in the Simulation Parameters dialog box (**Figure 33**). These define the source area, time stepping, profile times and ending criterion as indicated in Table 26.

Table 26 Problem 1 Simulation Control Parameters

Parameter	Rationale	Value
Radius of the NAPL Source, R_s	A "per unit area" simulation is desired, the value 0.5642 results in a 1.0 m^2 source area	0.5642 m
Simulation Ending Time	Simulate the release for 25 days, since gasoline is a low viscosity fluid and can reach the water table relatively rapidly in a permeable media.	25 days
Maximum Solution Time Step	Use a relatively small value, because only 25 days are simulated	0.1 day
Minimum Time Between Printed Time Steps	Use a value smaller that the minimum solution time step.	0.05 day

Five profiles times are used for the simulation. The times should be small, since the gasoline is expected to reach the water table relatively rapidly. Use times of 0.25, 0.5, 1.0, 2.0 and 5.0 days (6, 12, 24, 48 and 60 hours). HSSM-WIN requires at least one groundwater receptor be indicated. Here the receptor is arbitrarily located at (0.0,0.0).



SIMULATION CONTROL PARAMETERS

Radius of NAPL lens source (m). 5642
Radius multiplication factor 0000
Max NAPL saturation in NAPL lens . . .0000
Simulation ending time (d) 25.00
Maximum solution time step (d) 1000
Minimum time between printed time steps (d) .5000E-01

OILENS Simulation ending criterion
● User-specified time
○ NAPL lens spreading stops
○ Max contaminant mass flux into aquifer
○ Contaminant leached from lens
Fraction of mass remaining 0000

HSSM-T MODEL PARAMETERS

Percent max. contam't radius (%) 0000
Minimum output conc'n (mg/L) 0000
Beginning time (d) 0000
Ending time (d) 0000
Time increment (d) 0000

Data file:
C:\HSSM\X1STF.DAT

☐ Enable range checking

NAPL LENS PROFILES
Enter time (d) for each of up to 10 profiles

1	.2500
2	.5000
3	1.000
4	2.000
5	5.000
6	
7	
8	
9	
10	

Number of profiles 5

RECEPTOR WELL LOCATIONS
Enter coordinates for each of up to 6 wells

	X (m)	Y (m)
1	0.0	0.0
2		
3		
4		
5		
6		

Number of wells 1

Figure 33 Problem 1 completed Simulation Parameters dialog box

Problem 1 Model Results

The model is executed by entering the command

```
HSSM-KO X1STF.DAT
```

The saturation profiles from the simulation are shown in **Figure 34**. These profiles were drawn with the HSSM-PLT program. The depth of the sharp front increases with time and the first three profiles show uniform NAPL saturations. The last two profiles show varying NAPL saturations, because they occur at 48 and 60 hours which both are past the end of the release (24 hours).

With complete confidence in the accuracy of the input data, it could be assumed that the gasoline never reaches the water table. Most of the model parameters used in this example have been estimated from published tabulations. Rather than accepting the results of one simulation as being authoritative, several simulations should be run in order to get some feel for the effects of parameter variability. If the hydraulic conductivity was in fact 10 times greater than the average value of 0.75 m/d, the gasoline would flow deeper into the subsurface. Because of the constant head ponding condition assumed for this case, the gasoline would also flow faster. The constant head ponding condition does not specify the volume of gasoline which enters the soil; it only indicates that enough gasoline is supplied to maintain the 0.05 m ponding depth for one day. **Figure 35** shows the NAPL front position when the hydraulic conductivity is 7.5 m/d. By 25 days, the gasoline would reach 24 meters deep, if not for the water table 5.0 meters deep. From the **X2STF.HSS** file, the depth of 5 meters was reached within 9.8 hours.

This example has focussed on the role of the hydraulic conductivity in determining the depth of the gasoline. The effect of variation in other parameters can likewise be demonstrated. Some of the other uncertain parameters are the assumed release condition, moisture content, and capillary pressure parameters.

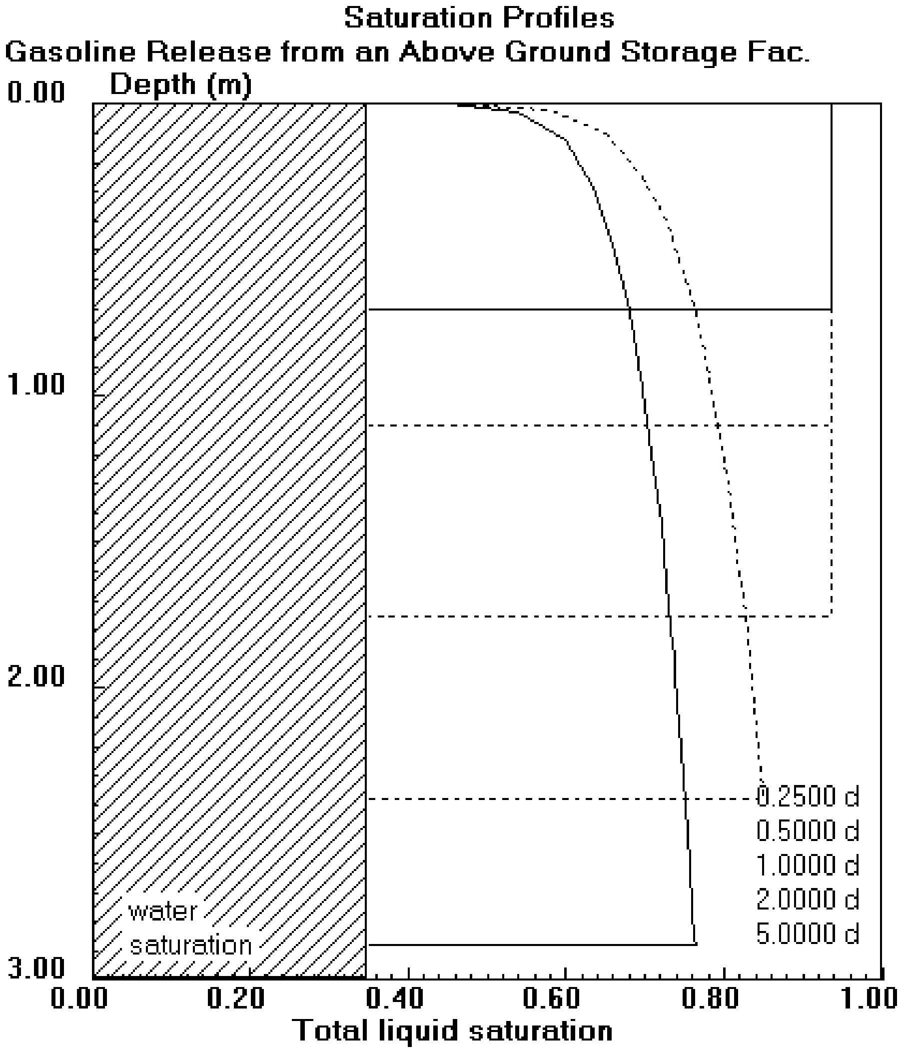


Figure 34 The storage tank example saturation profiles

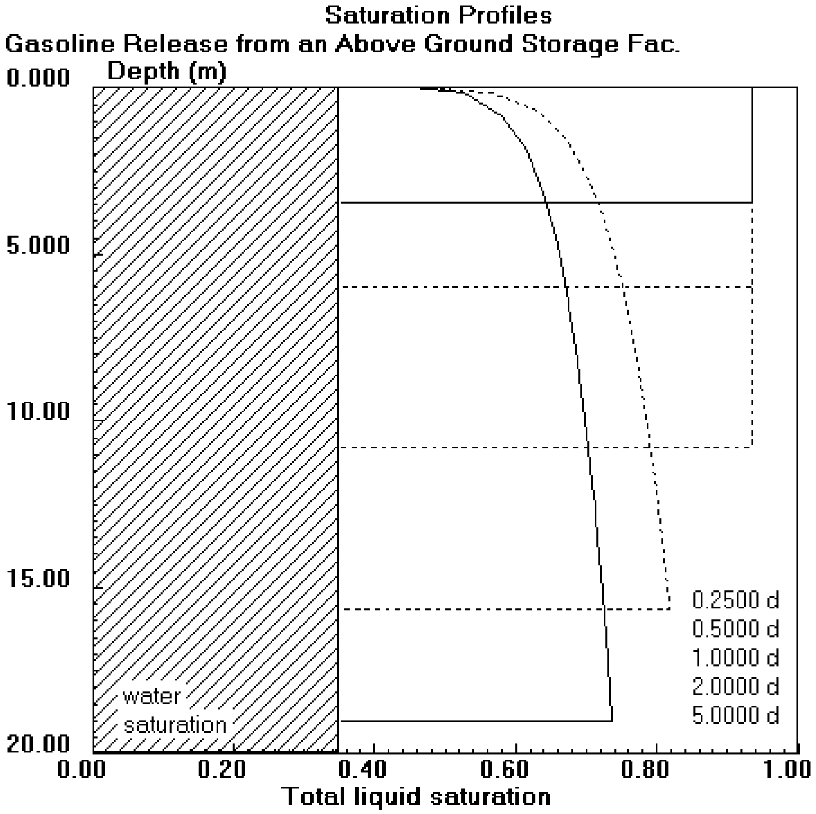


Figure 35 Storage tank facility example with increased conductivity

5.2 Problem 2: Transport of Gasoline Constituents in Ground Water to Receptor Locations

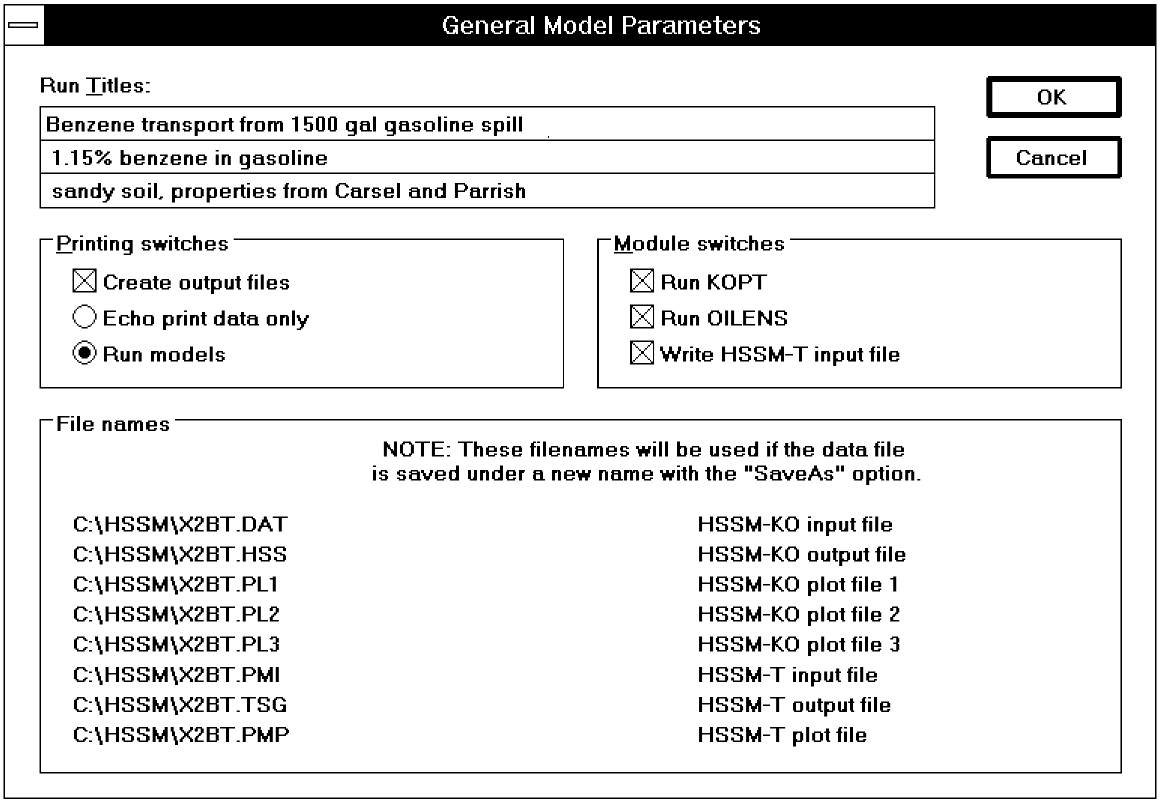
During a one-day period, 1500 gallons of gasoline leak from a tank surrounded by a circular berm of 2.0 meter radius. Benzene is believed to compose 1.15% by mass of the gasoline. The benzene concentration in the ground water at locations 25, 50, 75, 100, 125 and 150 meters away are needed to assess the impact of the spill. The soil is believed to be predominantly sand in the vicinity of the spill. The aquifer is 10 meters below the ground surface, and its saturated thickness is 15 meters.

Complete information for the site is not available so many of the HSSM parameters must be estimated. In the absence of better information, parameter values will be estimated from tabulations from the literature. The data set for this example will be organized according to the 4 dialog boxes for entering data in HSSM-WIN. The parameters for this example are found in the file **X2BT.DAT**, which is found on the HSSM-WIN distribution diskette. The file may be loaded and viewed according to the instructions in section 4.5.2 "Creating and Editing Input Data Sets."

The first of the boxes, "General Model Parameters," contains the run title, printing switches, module switches and the file names. For this example, the run title is

Benzene transport from 1500 gal gasoline release
Benzene 1.15% by mass of gasoline
sandy soil from Carsel and Parrish Data set

The "create output files" switch is checked in order to write the output files. For the first attempt at running a new data set, it is recommended to echo print the input data only and check the parameter values by reading the ***.HSS** output file. Each of the Module switches is checked, because all three of the HSSM modules are needed for estimating the receptor concentrations. At this point the names are of no concern as they are added automatically when the file is saved. The file name used for this simulation is **X2BT.DAT**. The completed dialog box appears as shown in **Figure 36**.



Run Titles:

Benzene transport from 1500 gal gasoline spill
1.15% benzene in gasoline
sandy soil, properties from Carsel and Parrish

Printing switches

☒ Create output files
○ Echo print data only
● Run models

Module switches

☒ Run KOPT
☒ Run OILENS
☒ Write HSSM-T input file

File names

NOTE: These filenames will be used if the data file
is saved under a new name with the "SaveAs" option.

C:\HSSM\X2BT.DAT	HSSM-KO input file
C:\HSSM\X2BT.HSS	HSSM-KO output file
C:\HSSM\X2BT.PL1	HSSM-KO plot file 1
C:\HSSM\X2BT.PL2	HSSM-KO plot file 2
C:\HSSM\X2BT.PL3	HSSM-KO plot file 3
C:\HSSM\X2BT.PMI	HSSM-T input file
C:\HSSM\X2BT.TSG	HSSM-T output file
C:\HSSM\X2BT.PMP	HSSM-T plot file

Figure 36 Problem 2 completed General Parameters dialog box

The second dialog box, "Hydrologic Parameters" contains the hydrologic and soil properties.

Hydrologic Properties

Standard properties of water are used for the simulation: density of 1.0 g/cm^3, viscosity of 1.0 cp, and surface tension of 65 dyne/cm. During infiltration, some of the air in the pore space is not displaced by either the water or the NAPL. It is assumed that during infiltration the maximum hydraulic conductivity to water is one-half of the saturated hydraulic conductivity. From this assumption, HSSM automatically determines the amount of air trapped in the pore space.

Recharge

The average annual recharge rate at the release site is estimated to be 50 cm/year. When converted into the required HSSM units of meters per day, the recharge rate is 0.0014 m/d.

Capillary Pressure Curve Model and the Porous Medium Properties

The tabulation of soil parameters developed by Carsel and Parrish (1988) will be used for the soil properties because of the relatively large number of samples used in developing the statistics for the sand classification. The parameters in Table 27 are taken from the tabulation (which is reproduced in Appendix 3.1).

Table 27 Problem 2 Hydraulic Properties

Parameter	Average value from Carsel and Parrish (1988)
Hydraulic conductivity, K_s	7.1 m/d
Residual water content, θ_{wr}	0.045
Saturated water content, θ_m	0.43
van Genuchten capillary parameter "α"	4.5 m^{-1}
van Genuchten capillary parameter "n"	2.68

These parameters form the basis for several of the other required input parameters on the "Hydrologic Parameters" dialog box. The parameter listed in Table 28 are derived from the soils data.

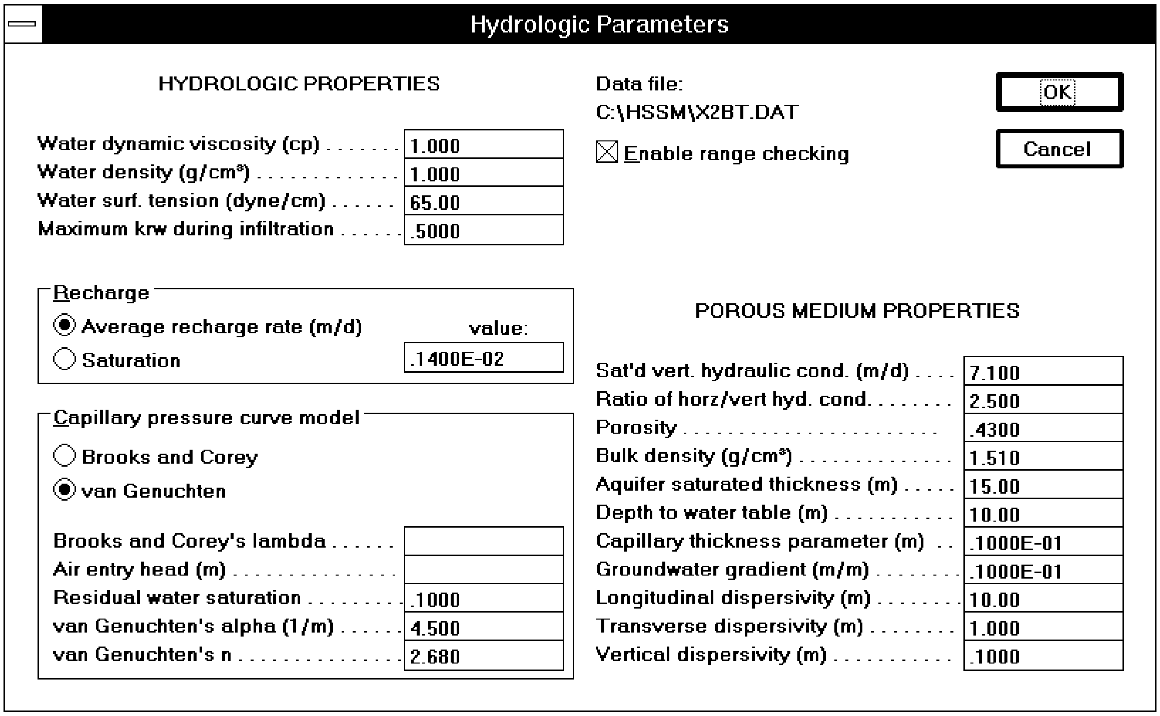
Table 28 Problem 2 Parameters Derived from the Hydraulic Properties

Parameter	Rationale	Value
Residual water saturation, S_{wr}	HSSM requires residual saturation to be entered, rather than residual moisture content. $S_{wr} = \theta_{wr} / \theta_m$	0.10 (0.045/0.43)
Ratio of horizontal to vertical conductivity	The sandy soil is assumed to be only slightly anisotropic.	2.5
Porosity, η	The porosity is taken as being equal to the saturated water content.	0.43
Bulk density, ρ_b	In terms of porosity and solid density, the bulk density is $\rho_b = \rho_s(1 - \eta)$.	1.51 g/cm^3 2.65 g/cm^3 (1 - 0.43)

The aquifer saturated thickness is 15.0 meters, and the depth to the water table is 10.0 meters. For this simulation, no smear zone is included; so the NAPL is allowed to spread out freely along the water table. Thus the capillary thickness parameter is set to a minimum value of 0.01 m.

The ground water gradient is estimated to be 1 foot per hundred or 0.01. The longitudinal dispersivity is taken as 10 meters. This value follows from the rule of thumb that says that the longitudinal dispersivity could be one tenth the distance to the receptor point (100 m). The horizontal transverse dispersivity is assumed to be 1 meter and the vertical transverse dispersivity is assumed to be 0.1 m.

At this point the "Hydrologic Parameters" dialog box of HSSM-WIN can be completely filled in (**Figure 37**).



HYDROLOGIC PROPERTIES

Water dynamic viscosity (cp) 1.000
Water density (g/cm^3) 1.000
Water surf. tension (dyne/cm) 65.00
Maximum krw during infiltration ...... .5000

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

Recharge
● Average recharge rate (m/d) value: .1400E-02
○ Saturation

Capillary pressure curve model
○ Brooks and Corey
● van Genuchten

Brooks and Corey's lambda ......
Air entry head (m) ....
Residual water saturation .... .1000
van Genuchten's alpha (1/m) 4.500
van Genuchten's n 2.680

POROUS MEDIUM PROPERTIES

Sat'd vert. hydraulic cond. (m/d) 7.100
Ratio of horz/vert hyd. cond. 2.500
Porosity .... .4300
Bulk density (g/cm^3) 1.510
Aquifer saturated thickness (m) 15.00
Depth to water table (m) 10.00
Capillary thickness parameter (m) .. .1000E-01
Groundwater gradient (m/m) .... .1000E-01
Longitudinal dispersivity (m) 10.00
Transverse dispersivity (m) 1.000
Vertical dispersivity (m) .... .1000

Figure 37 Problem 2 completed Hydrologic Properties dialog box

Hydrocarbon Phase Properties

The first group of parameters is used to describe the properties of the NAPL itself, which is assumed to be an inert oily phase. The density and viscosity of gasoline are typically near 0.74 g/cm^3 and 0.45 cp, respectively. The solubility of the NAPL is arbitrarily taken as 10 mg/l. A small amount of the NAPL phase will dissolve during the simulation, but this amount has little effect on the dissolved constituent of interest. Residual NAPL saturations are specified for the aquifer (0.15) and the vadose zone (0.05). These values are estimates, but reflect the fact that the residual in the aquifer is likely to be higher than that in the vadose zone (Wilson et al., 1990). The soil/water partition coefficient for the NAPL phase is taken to be 0.83. The NAPL or "oil" surface tension is assumed to be about half of the water/air surface tension, σ_{ao} or 35 dyne/cm.

Dissolved Constituent Properties

Since the object of the simulation is to estimate down gradient concentrations of a chemical of interest, the dissolved constituent exists box is checked. The initial constituent concentration (of benzene) is calculated from its mass percentage in the gasoline. The dissolved constituent check box is selected to tell HSSM that a dissolved constituent of the NAPL should be simulated.

Since the benzene is present in the gasoline at a mass fraction of 1.14% and the density of the gasoline is 0.72 g/cm^3, the initial concentration of benzene in the gasoline is

$$8208\,mg/L \quad = \quad \frac{1.14\,\%}{100}\,(0.72\,g/cm^3)\,(1000\,cm^3/L)\,(1000\,mg/g) \tag{18}$$

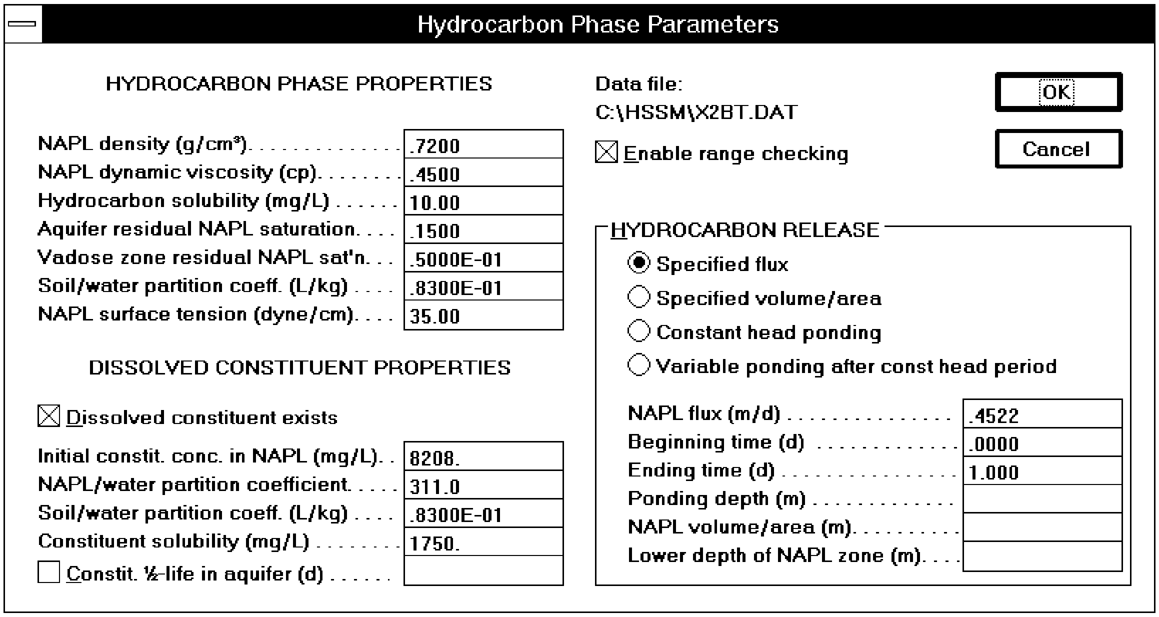
The Oil/Water (NAPL/Water) partition coefficient, K_o, will be assumed to be equal to 311 as determined from the RAOULT utility (Appendices 3.2 and 6). The benzene partition coefficient between the soil and water, K_d, is 0.083 L/kg. The value is determined by multiplying the assumed fraction organic carbon (0.001) by the value of K_{oc} (83). The value of K_{oc} is taken from Table 98 in Appendix 3.2. The water solubility of benzene is about 1750 mg/l. This value is an absolute limiting value for the simulation. The actual solubility of benzene in the gasoline is determined by the partition coefficient. No degradation of the benzene will be assumed for the HSSM-T model, so the half-life check box is unchecked.

Hydrocarbon Release

The release in this example is given as a volume released during a certain time interval. The appropriate release definition for this situation is the specified flux release. The required input parameters are the beginning time in days and the ending time in days, and the NAPL flux in meters per day. The beginning time is 0.0 days and the ending time is 1.0 days. The NAPL flux, q_o, is calculated by dividing the release volume by the source area and the duration.

$$q_o \quad = \quad 0.4522\, m/d \quad = \quad \frac{1500\, gal \left(\dfrac{ft^3}{7.5\, gal}\right) \left(\dfrac{0.3048m}{ft}\right)^3}{\left(\pi\ \ (2.0\, m)^2\right) \ \ 1.0\, day} \tag{19}$$

The completed dialog box is shown in **Figure 38**.



HYDROCARBON PHASE PROPERTIES

NAPL density (g/cm³)	.7200
NAPL dynamic viscosity (cp)	.4500
Hydrocarbon solubility (mg/L)	10.00
Aquifer residual NAPL saturation	.1500
Vadose zone residual NAPL sat'n.	.5000E-01
Soil/water partition coeff. (L/kg)	.8300E-01
NAPL surface tension (dyne/cm)	35.00

DISSOLVED CONSTITUENT PROPERTIES

☒ Dissolved constituent exists

Initial constit. conc. in NAPL (mg/L)	8208.
NAPL/water partition coefficient	311.0
Soil/water partition coeff. (L/kg)	.8300E-01
Constituent solubility (mg/L)	1750.
☐ Constit. ½-life in aquifer (d)	

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

HYDROCARBON RELEASE

● Specified flux
○ Specified volume/area
○ Constant head ponding
○ Variable ponding after const head period

NAPL flux (m/d)	.4522
Beginning time (d)	.0000
Ending time (d)	1.000
Ponding depth (m)	
NAPL volume/area (m)	
Lower depth of NAPL zone (m)	

Figure 38 Problem 2 completed Hydrocarbon Phase Properties dialog box

Simulation Control Parameters

A number of parameters interact to control the various aspects of the simulation. These are listed in Table 29.

Table 29 Problem 2 Simulation Control Parameters		
Parameter	**Rationale**	**Value**
Radius of the NAPL source, R_s	From the problem definition	2.0 meters
Radius multiplication factor	Suggested value	1.001
Maximum NAPL saturation in the lens, $S_{o(max)}$	Estimated from the NTHICK utility described in Appendix 7	0.3260
Simulation ending time	A time much greater than that expected for the NAPL lens to form	2500 days
Maximum solution time step	Limit of approximately less than 1 month	20 days
Minimum time between printed time steps and mass balance checks	The model can produce output on very small time intervals, such information is of little usefulness.	0.1 days

OILENS Simulation Ending Criterion

The fourth option, "contaminant leached from lens," is chosen for the ending condition as this is the only option that allows the HSSM-T model to be run. The fraction of mass remaining is chosen to be 0.01. The OILENS portion of HSSM-KO will terminate when less than 1% of the mass that has entered the lens over the length of the simulation remains in the lens. The other 99% will have been leached into the ground water. The chemical constituent will still exist below the source in the vadose zone. This amount of chemical is contained in the NAPL phase as residual saturation, and it never enters the lens.

HSSM-T Model Parameters

Many previously entered parameters are used by HSSM-T. The remaining parameters are listed in Table 30.

Table 30 Problem 2 HSSM-T Model Parameters

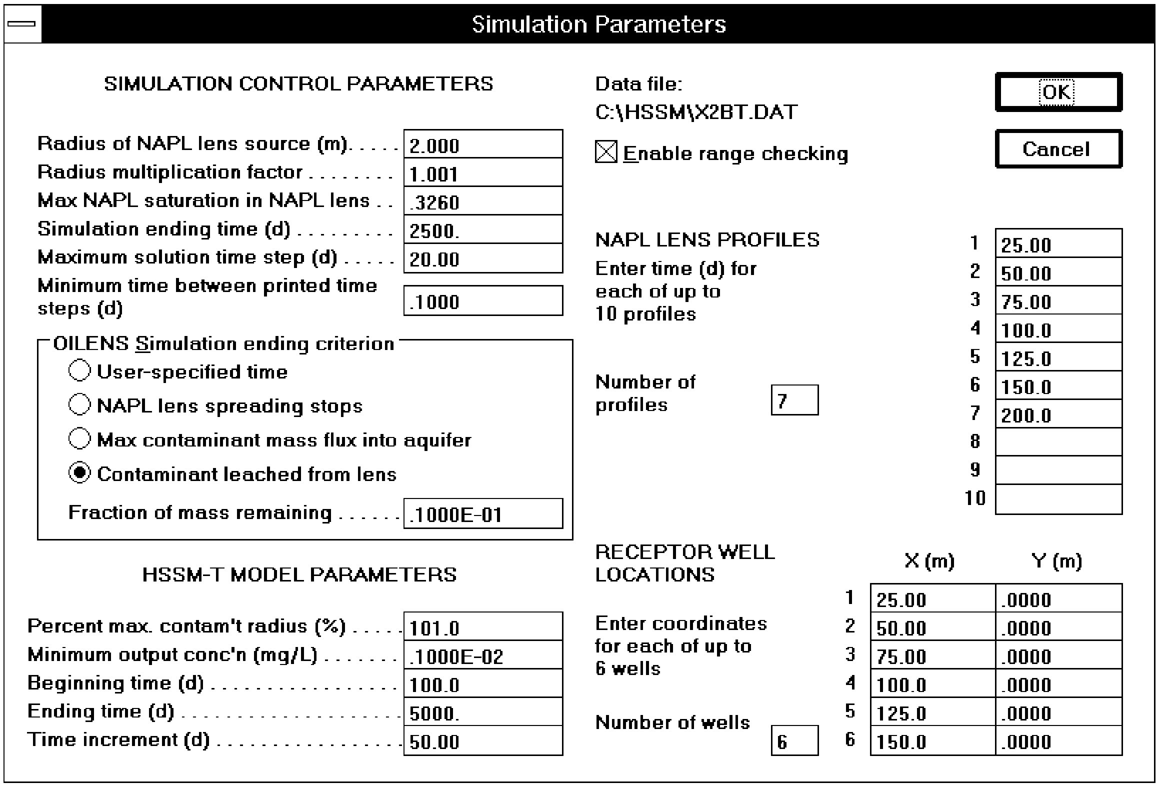
Parameter	Rationale	Value
Percent maximum contaminant radius	The radius that occurs when the mass flux to the aquifer is maximum should be used. The value 101 is a flag that triggers this selection.	101
Minimum output concentration	The minimum concentration that HSSM-T will report. A non-zero value is required for HSSM-T to function properly.	0.001 mg/l
Beginning time	Arbitrary value that will be overridden by a successful HSSM-T simulation	100 days
Ending time	Arbitrary value that will be overridden by a successful HSSM-T simulation	5000 days
Time increment	A 50-day time increment usually produces smooth concentration history curves	50 days

NAPL Lens Profiles

HSSM can output profiles at various times during the simulation. The profiles represent the amount of NAPL in the vadose zone pore space and the configuration of the NAPL lens. Because the motion of the gasoline is relatively rapid, the profiles should be clustered toward the release time. To catch the NAPL as it moves through the sandy vadose zone, for example, profile times less than about 1 day are needed. In this example, however, the lens configuration is of more interest and seven somewhat later profile times are selected: 25, 50, 75, 100, 125, 150 and 200 days.

Receptor Well Locations

The six receptor locations for this simulation are at 25, 50, 75, 100, 125 and 150 meters away from the center of the source, taken longitudinally in the flow direction. The completed dialog box is shown in **Figure 39**.



SIMULATION CONTROL PARAMETERS

Radius of NAPL lens source (m). 2.000
Radius multiplication factor 1.001
Max NAPL saturation in NAPL lens . . .3260
Simulation ending time (d) . . . . 2500.
Maximum solution time step (d) 20.00
Minimum time between printed time steps (d) .1000

OILENS Simulation ending criterion
○ User-specified time
○ NAPL lens spreading stops
○ Max contaminant mass flux into aquifer
● Contaminant leached from lens
Fraction of mass remaining 1000E-01

HSSM-T MODEL PARAMETERS

Percent max. contam't radius (%) 101.0
Minimum output conc'n (mg/L) 1000E-02
Beginning time (d) 100.0
Ending time (d) . . . . 5000.
Time increment (d) 50.00

Data file:
C:\HSSM\X2BT.DAT

☒ Enable range checking

NAPL LENS PROFILES
Enter time (d) for each of up to 10 profiles

Number of profiles 7

1	25.00
2	50.00
3	75.00
4	100.0
5	125.0
6	150.0
7	200.0
8	
9	
10	

RECEPTOR WELL LOCATIONS
Enter coordinates for each of up to 6 wells

Number of wells 6

	X (m)	Y (m)
1	25.00	.0000
2	50.00	.0000
3	75.00	.0000
4	100.0	.0000
5	125.0	.0000
6	150.0	.0000

Figure 39 Problem 2 completed Simulation Control dialog box parameters

Each graph generated by HSSM for this data set was shown previously in **Figure 23** to **Figure 28**. This example shows typical behavior for gasoline releases. There is relatively rapid flow and transport in the vadose zone followed by the formation and decay of a NAPL lens at the water table. Subsequent leaching of the chemical constituent of the NAPL (benzene) causes contamination of the aquifer. The time scales for lens formation and decay, leaching, and transport to the 150 m receptor are on the order of 1 year, 4 years, and 11 years, respectively.

Section 6 Contents of the Output Files

Although two graphical user interfaces are provided with HSSM, much of the useful and necessary information produced by the model is not contained on the graphs produced by these software packages. The main output files of the HSSM-KO and HSSM-T programs contain a summary of the input data and model results. The following tables describe each part of these files, along with excerpts from the output files. Several complete sets of output files are distributed on the HSSM-2 diskette.

6.1 HSSM-KO Output File

Table 31 outlines the contents of the HSSM-KO output file which has the extension **.HSS**. The output file consists of a series of tables which contain the results from the simulation.

Table 31 HSSM Main Output File Contents

Table Title	Contents
Input Data	1. Echo print of the input data. 2. Parameters calculated directly from input data. 3. Water/air and NAPL/air capillary pressure curves used in the model.
Location of the Oil Front	Position of the NAPL front during the simulation.
Location of the Constituent Front	Position of the chemical constituent of interest during the simulation.
OILENS Model Output--Oil Lens Description	Description of the NAPL lens during the simulation.
OILENS Model Output--Aqueous Contaminants	Description of leaching of aqueous contaminants during the simulation.
Saturation and Concentration Profile	Variation with depth of vadose zone saturations and concentrations at a user-specified time.
Radial Profile Through the Lens	Variation with radius of the top and bottom of the OILENS at a user-specific time.
KOPT/OILENS Postprocessing	Summary information from the simulation.
HSSM--Run Information	Information on the numerical techniques used in the simulation.

If the model executes with no catastrophic errors, then the HSSM-KO output file is ended with the message:

```
*********************
SUCCESSFUL EXECUTION
*********************
```

Each component of the output file is described in further detail below. For each table in the output file, the column headings and their meanings are described. An excerpt from the **.HSS** file follows each description.

Table 32 Input Data

Purpose: To provide an echo printing of the input data set and print out the results of preliminary calculations

Section	Contents
1	Echo printing of input data so the user can assure that the intended parameter values have been entered.
2	Model parameters calculated from the input data.
3	Air/water and air/NAPL capillary pressure curves used in the simulation.

```
**************************************************
HSSM            HYDROCARBON SPILL SIMULATION MODEL
**************************************************
KOPT            KINEMATIC OILY POLLUTANT TRANSPORT
OILENS          RADIAL OIL LENS MOTION
TSGPLUME        TRANSIENT SOURCE GAUSSIAN PLUME
**************************************************
Benzene transport from 1500 gal gasoline spill
 1.15% benzene in gasoline
 sandy soil, properties from Carsel and Parrish


     INPUT DATA
     ==========

     DATA FILES:
      HSSM-KO INPUT:     x2bt.dat
      HSSM-KO OUTPUT:    x2bt.HSS
      HSSM-KO PLOT 1:    x2bt.PL1
      HSSM-KO PLOT 2:    x2bt.PL2
      HSSM-KO PLOT 3:    x2bt.PL3
      HSSM-T INPUT:      x2bt.PMI
      HSSM-T OUTPUT:     x2bt.TSG
      HSSM-T PLOT:       x2bt.PMP
     INTERFACE FLAG             = D
     WRITING CRITERIA           =          1
     KOPT RUN FLAG              =          1
     DISSOLVED CONSTITUENT FLAG  =          1
     OILENS RUN FLAG            =          1
     TSGPLUME RUN FLAG          =          1

     CONSTANTS & MATRIX PROPERTIES...........
     SAT. VERT. HYD.CONDUCTIVITY =  7.100     (M/D)
     RATIO OF HORIZONTAL TO
     VERTICAL CONDUCTIVITY      =  2.500     (*)
     RELATIVE PERMEABILITY INDEX =          2 (*)
     POROSITY                   =  .4300     (*)
     RESIDUAL WATER SATURATION   =  .1000     (*)
```

```
VAN GENUCHTEN'S N           =  4.500     (*)

WATER EVENT CHARACTERISTICS.............
DYNAMIC VISCOSITY           =  1.000     (CP)
DENSITY                     =  1.000     (G/CC)
RAIN TYPE : 1-FLUX 2-SAT.   =          1 (*)
WATER FLUX OR SATURATION    =  .1400E-02 (M/D OR *)
MAX KRW DURING INFILTRATION =  .5000     (*)
DEPTH TO WATER TABLE        =  10.00     (M)

POLLUTANT EVENT CHARACTERISTICS.........
DYNAMIC VISCOSITY           =  .4500     (CP)
DENSITY                     =  .7200     (G/CC)
RESIDUAL NAPL SATURATION    =  .5000E-01 (*)
OIL LOADING TYPE            =          1 (*)

CAPILLARY SUCTION PARAMETERS............
VAN GENUCHTENS ALPHA        =  2.680     (1/M)
WATER SURFACE TENSION       =  65.00     (DYNE/CM)
OIL SURFACE TENSION         =  35.00     (DYNE/CM)

FLUX LOADING RATE           =  .4522     (M/D)
BEGINNING TIME              =  .0000     (D)
ENDING TIME                 =  1.000     (D)

DISSOLVED CONSTITUENT PARAMETERS........
INITIAL CONC. IN NAPL       =  8208.     (MG/L)
NAPL/WATER PARTITION COEF.  =  311.0     (*)
SOIL/WATER PARTITION COEF.  =  .8300E-01 (L/KG)
SOIL/WATER (HYDROCARBON)    =  .8300E-01 (L/KG)
BULK DENSITY                =  1.510     (G/CC)

OILENS SUBMODEL PARAMETERS..............
RADIUS OF POLLUTANT SOURCE  =  2.000     (M)
RADIUS MULTIPLYING FACTOR   =  1.001     (*)
THICKNESS OF CAP. FRINGE    =  .1000E-01 (M)
AQUIFER'S VERT DISPERSIVITY =  .1000     (M)
GROUNDWATER GRADIENT        =  .1000E-01 (*)
NAPL RESIDUAL IN AQUIFER    =  .1500     (*)
MAX NAPL SATURATION IN LENS =  .3260     (*)
WATER SOLUBILITY CONTAMINANT=  1750.     (MG/L)
WATER SOLUBILITY OF OIL     =  10.00     (MG/L)

SIMULATION PARAMETERS...................
SIMULATION ENDING TIME      =  2500.     (D)
MAXIMUM RKF TIME STEP       =  20.00     (D)
MIN. TIME BETWEEN PRINTING  =  .1000     (D)
ENDING CRITERIA             =          4 (*)
FACTOR FOR ENDING CRITERIA 4=  .1000E-01 (*)

PROFILES................................
NUMBER OF PROFILES          =          7 (*)
AT TIMES:                                (D)
     25.0000      50.0000      75.0000
    100.0000     125.0000     150.0000
    200.0000

TSGPLUME MODEL PARAMETERS...............
LONGITUDINAL DISPERSIVITY      10.00     (M)
```

```
TRANSVERSE DISPERSIVITY        1.000     (M)
PERCENT MAX. RADIUS            101.0     (M)
MINIMUM OUTPUT CONC.           .1000E-02 (MG/L)
CONSTITUENT HALF LIFE          .0000     (D)
NUMBER OF RECEPTOR LOCATIONS           6 (*)
BEGINNING TIME (D)             100.0     (D)
ENDING TIME (D)                5000.     (D)
TIME INCREMENT (D)             50.00     (D)
AQUIFER THICKNESS (M)          15.00     (M)

RECEPTOR LOCATIONS
              X          Y
      25.00      .0000
      50.00      .0000
      75.00      .0000
      100.0      .0000
      125.0      .0000
      150.0      .0000


LEGEND
======
(*)       DIMENSIONLESS OR NOT APPLICABLE
(M)       METERS
(D)       DAYS
(CP)      CENTIPOISE  1.0 CP = 0.01 GR/CM/SEC
(M/D)     METERS PER DAY
(DYNE/CM) DYNE PER CENTIMETER
(MG/L)    MILLIGRAMS PER LITER
(L/KG)    LITERS PER KILOGRAM SOIL
(G/CC)    GRAMS PER CUBIC CENTIMETER



***END OF INPUT DATA***
```

Parameters calculated directly from the input data follow the echo printing of the input data set:

```
CALCULATED PARAMETERS..................
SAT VERT NAPL  CONDUCTIVITY =  11.36     (M/D)
AREA OF THE SOURCE          =  12.57     (M^2)
APPROX. BROOKS AND COREY
LAMBDA                      =  2.064     (*)
AIR ENTRY HEAD              =  .2759     (M)
TRAPPED AIR SATURATION      =  .1442     (*)
WATER SATURATION            =  .2049     (*)
WATER FLUX                  =  .1400E-02 (M/D)
MAX. OIL CONDUCTIVITY       =  3.157     (M/D)
POLLUTANT VOLUME FLUX        =  .4522     (M/D)
TOTAL OIL LOADING, VOL/AREA =  .4522     (M)
TOTAL OIL MASS              =  4091.     (KG)
TOTAL CONSTITUENT MASS      =  46.64     (KG)
```

The estimated capillary pressure curves for air/water and air/NAPL follow the input data in the **name.HSS** file:

```
WATER-AIR, NAPL-AIR CAPILLARY PRESSURE CURVE
********************************************

WATER or NAPL CAPILLARY       CAPILLARY
SATURATION    HEAD (CM WATER) HEAD (CM NAPL)
===================================================

     .1200         1.7438         1.3041
     .1400         1.2464          .9322
     .1600         1.0242          .7659
     .1800          .8909          .6663
     .2000          .7997          .5980
     .2200          .7321          .5475
     .2400          .6794          .5081
     .2600          .6368          .4763
     .2800          .6015          .4499
     .3000          .5716          .4275
     .3200          .5458          .4082
     .3400          .5233          .3913
     .3600          .5034          .3765
     .3800          .4856          .3632
     .4000          .4697          .3512
     .4200          .4552          .3404
     .4400          .4420          .3306
     .4600          .4300          .3216
     .4800          .4189          .3132
     .5000          .4086          .3056
     .5200          .3990          .2984
     .5400          .3901          .2918
     .5600          .3818          .2856
     .5800          .3740          .2797
     .6000          .3667          .2743
     .6200          .3598          .2691
     .6400          .3533          .2642
     .6600          .3471          .2596
     .6800          .3413          .2552
     .7000          .3357          .2511
     .7200          .3304          .2471
     .7400          .3254          .2433
     .7600          .3206          .2397
     .7800          .3160          .2363
     .8000          .3116          .2330
     .8200          .3073          .2298
     .8400          .3033          .2268
     .8600          .2994          .2239
     .8800          .2957          .2211
     .9000          .2920          .2184
     .9200          .2886          .2158
     .9400          .2852          .2133
     .9600          .2820          .2109
     .9800          .2789          .2086
    1.0000          .2759          .2063
```

Table 33 Location of the NAPL Front

Purpose: A summary of the NAPL distribution in the vadose zone.

Column	Column Heading	Contents
1	Step	The number of time steps completed. These numbers are usually not consecutive, because a minimum printing interval should be chosen.
2	Time (D)	The time in days since the beginning of the simulation.
3	Depth (M)	The depth of the sharp front at the leading edge of the infiltrating NAPL.
4	Saturation	The NAPL saturation at the front; NAPL saturations behind the front are often lower than this value, as can be seen on the saturation profiles.
5	Flux (M/D)	NAPL flux at the front.
6	Runoff (KG)	Runoff is produced when a NAPL flux boundary condition is specified and the flux is greater than the maximum dynamic flux allowed by the Green-Ampt model with zero ponding head.
7	Mass (KG)	NAPL mass added to the profile per square meter.
8	Ponding (M)	The surface ponding depth of NAPL.

NOTE: This output table is produced only up until a NAPL lens forms. At that time the OILENS model output is produced.

```
       **************************************************
                    LOCATION OF THE NAPL FRONT
       **************************************************
       Benzene transport from 1500 gal gasoline spill
        1.15% benzene in gasoline
        sandy soil, properties from Carsel and Parrish

                                      NAPL
                 ------------------------------------------------
 STEP    TIME     DEPTH  SATURATION     FLUX     RUNOFF    MASS    PONDING
         (D)       (M)       (*)        (M/D)    (KG)      (KG)      (M)
============================================================================

    1     .0000     .0000     .3957     .4522     .0000     .0000
    4     .2000     .5315     .3957     .4522 .0000     818.3             .0000
    5     .3000     .7972     .3957     .4522 .0000     1227.             .0000
    7     .5000    1.3287     .3957     .4522 .0000     2046.             .0000
    8     .6000    1.5944     .3957     .4522 .0000     2455.             .0000
    9     .7000    1.8602     .3957     .4522 .0000     2864.             .0000
   10     .8000    2.1259     .3957     .4522 .0000     3273.             .0000
   11     .9000    2.3917     .3957     .4522 .0000     3682.             .0000
   13    1.0107    2.6858     .3957     .4522 .0000     4091.             .0000
   23    1.1182    2.9715     .3957     .4522 .0000     4091.             .0000
   29    1.2248    3.2548     .3957     .4522 .0000     4091.             .0000
   33    1.3330    3.5423     .3957     .4522 .0000     4092.             .0000
   38    1.4399    3.8024     .3710     .3510 .0000     4092.             .0000
   41    1.5691    4.0598     .3472     .2703 .0000     4091.             .0000
   43    1.6771    4.2426     .3320     .2266 .0000     4091.             .0000
   45    1.8050    4.4325     .3175     .1900 .0000     4091.             .0000
   47    1.9668    4.6423     .3029     .1577 .0000     4091.             .0000
   49    2.1530    4.8527     .2895     .1317 .0000     4091.             .0000
   50    2.2657    4.9677     .2826     .1197 .0000     4091.             .0000
   51    2.3909    5.0866     .2758     .1087 .0000     4091.             .0000
   52    2.5290    5.2086     .2692     .0986 .0000     4091.             .0000
   53    2.6809    5.3332     .2627     .0894 .0000     4091.             .0000
   54    2.8478    5.4605     .2564     .0811 .0000     4091.             .0000
   55    3.0310    5.5905     .2503     .0736 .0000     4091.             .0000
```

{Intermediate results omitted}

```
   67    7.0717    7.3052     .1892     .0234 .0000     4089.             .0000
   68    7.6604    7.4685     .1848     .0212 .0000     4089.             .0000
   69    8.2492    7.6205     .1809     .0194 .0000     4089.             .0000
   70    8.8379    7.7628     .1774     .0179 .0000     4089.             .0000
   71    9.5411    7.9217     .1736     .0163 .0000     4089.             .0000
   72   10.3414    8.0901     .1697     .0148 .0000     4089.             .0000
   73   11.1417    8.2470     .1663     .0136 .0000     4089.             .0000
   74   12.0723    8.4171     .1626     .0123 .0000     4089.             .0000
   75   13.1191    8.5947     .1590     .0112 .0000     4089.             .0000
   76   14.1658    8.7601     .1557     .0102 .0000     4089.             .0000
   77   15.3753    8.9379     .1524     .0093 .0000     4089.             .0000
   78   16.7325    9.1231     .1490     .0084 .0000     4088.             .0000
   79   18.0897    9.2953     .1460     .0077 .0000     4088.             .0000
   80   19.4469    9.4562     .1433     .0071 .0000     4088.             .0000
   81   21.0820    9.6370     .1403     .0064 .0000     4087.             .0000
   82   22.9444    9.8283     .1372     .0058 .0000     4087.             .0000
   83   24.6391    9.9905     .1348     .0054 .0000     4086.             .0000
```

Table 34 Location of the Constituent Front

Purpose: A summary of the vadose zone distribution of the dissolved constituent.

Column	Column Heading	Contents
1	Step	The number of time steps completed.
2	Time	The time in days since the beginning of the simulation.
3	Depth-Upper	The depth in meters of the leading edge of the constituent.
4	Depth-Lower	The depth in meters of the trailing edge of the constituent
5	Conc-water	The water phase concentration of the constituent at the leading edge.
6	Mass	The total mass of the constituent in the vadose zone.

NOTE: This output table is produced only up until a NAPL lens forms. At that time the OILENS model output takes over.

```
        **************************************************
                     LOCATION OF THE CONSTITUENT FRONT
        **************************************************
        Benzene transport from 1500 gal gasoline spill
         1.15% benzene in gasoline
         sandy soil, properties from Carsel and Parrish

                                   CONSTITUENT
                  --------------------------------------
  STEP    TIME          DEPTHS     CONC-WATER MASS
                    LOWER     UPPER
 =======================================================

     4     .2000     .5294     .0000   26.3920 9.329
     5     .3000     .7941     .0000   26.3920 13.99
     7     .5000    1.3235     .0000   26.3920 23.32
     8     .6000    1.5882     .0000   26.3920 27.99
     9     .7000    1.8529     .0000   26.3920 32.65
    10     .8000    2.1176     .0000   26.3920 37.32
    11     .9000    2.3823     .0000   26.3920 41.98
    13    1.0107    2.6753     .0000   26.3920 46.64
    23    1.1182    2.9598     .0000   26.3920 46.65
    29    1.2248    3.2419     .0000   26.3920 46.65
    33    1.3330    3.5283     .0001   26.3920 46.65
    38    1.4399    3.7864     .0001   26.3920 46.65
    41    1.5691    4.0416     .0001   26.3920 46.65
    43    1.6771    4.2226     .0001   26.3920 46.65
    45    1.8050    4.4107     .0002   26.3920 46.64
    47    1.9668    4.6184     .0002   26.3920 46.64
    49    2.1530    4.8265     .0002   26.3920 46.64
    50    2.2657    4.9403     .0003   26.3920 46.64
    51    2.3909    5.0578     .0003   26.3920 46.64
    52    2.5290    5.1784     .0003   26.3920 46.64
    53    2.6809    5.3015     .0003   26.3920 46.64
    54    2.8478    5.4273     .0004   26.3920 46.64
    55    3.0310    5.5556     .0004   26.3920 46.64
    56    3.2321    5.6864     .0005   26.3920 46.64
    57    3.4528    5.8197     .0005   26.3920 46.64

{Intermediate results omitted}
    65    6.0533    6.9350     .0010   26.3920 46.63
    66    6.5365    7.0879     .0011   26.3920 46.63
    67    7.0717    7.2452     .0012   26.3920 46.62
    68    7.6604    7.4057     .0013   26.3920 46.62
    69    8.2492    7.5551     .0015   26.3920 46.62
    70    8.8379    7.6949     .0016   26.3920 46.62
    71    9.5411    7.8510     .0017   26.3920 46.62
    72   10.3414    8.0163     .0019   26.3920 46.62
    73   11.1417    8.1702     .0021   26.3920 46.62
    74   12.0723    8.3370     .0022   26.3920 46.62
    75   13.1191    8.5113     .0025   26.3920 46.62
    76   14.1658    8.6733     .0027   26.3920 46.62
    77   15.3753    8.8475     .0029   26.3920 46.62
    78   16.7325    9.0288     .0032   26.3920 46.62
    79   18.0897    9.1973     .0035   26.3920 46.62
    80   19.4469    9.3547     .0037   26.3920 46.61
    81   21.0820    9.5316     .0041   26.3920 46.61
```

Table35 OILENS Model Output--NAPL Lens Description

Purpose: A summary of the NAPL lens configuration.

Column	Column Heading	Contents
1	Step	The number of time steps completed.
2	Time	The time in days since the beginning of the simulation.
3	Lens Height	The height in meters of the NAPL lens above the spreading zone.
4	Lens Radius	The radius in meters of the NAPL lens.
5	Lens Volume	The volume of NAPL in the lens in cubic meters.
6	Residual Volume	The volume of NAPL in cubic meters trapped at residual above and below the lens
7	Volume Losses	The cumulative volume of NAPL lost to dissolution in cubic meters.
8	Cumulative Inflow	The cumulative volume inflow of NAPL to the lens in cubic meters.
9	Percent Volume Error	The percent error in calculated NAPL volume as compared with the cumulative NAPL inflow to the lens. This volume balance does not include NAPL in the vadose zone.

```
               **************************************************
               *    OILENS MODEL OUTPUT--OIL LENS DESCRIPTION   *
               **************************************************
               Benzene transport from 1500 gal gasoline spill
                1.15% benzene in gasoline
                sandy soil, properties from Carsel and Parrish

                  LENS     LENS     LENS     RESIDUAL VOLUME   CUM.    PERCENT
          TIME    HEIGHT   RADIUS   VOLUME   VOLUME   LOSSES   INFLOW   VOLUME
   STEP  (DAYS)  (METERS) (METERS)  (CU.M.)  (CU.M.)  (CU.M.)  (CU.M.)  ERROR

==============================================================================


          *** OIL FILLING CAPILLARY FRINGE
          *** TIME                           =    24.6391
          *** OIL SATURATION IN LENS         =      .3260
          *** CAPILLARY FRINGE OIL THICKNESS =      .0100

    85    24.90    .0000     2.00      .02      .00      .00      .02      .20
    93    25.01    .0011     2.02      .02      .00      .00      .02      .14
    95    25.13    .0022     2.05      .03      .00      .00      .03      .11
    96    25.27    .0035     2.08      .04      .00      .00      .04      .08
    97    25.42    .0047     2.10      .05      .00      .00      .05      .06
    98    25.68    .0069     2.15      .07      .00      .00      .07      .03
   102    25.79    .0077     2.17      .08      .00      .00      .08      .03
   115    25.92    .0086     2.20      .08      .00      .00      .08      .03
   118    26.05    .0096     2.22      .09      .00      .00      .09      .02
   120    26.21    .0107     2.25      .10      .00      .00      .10      .02
```

{Intermediate results omitted}

```
   241   807.00    .0045    16.35     1.99      .58      .09     2.66      .04
   242   827.00    .0044    16.44     1.99      .59      .09     2.67      .05
   243   847.00    .0042    16.52     1.98      .60      .09     2.67      .06
   244   867.00    .0041    16.59     1.97      .60      .10     2.67      .07
   245   887.00    .0040    16.67     1.97      .61      .10     2.68      .08
   246   907.00    .0039    16.74     1.96      .62      .10     2.68      .10
   247   927.00    .0038    16.81     1.96      .62      .11     2.68      .11
   248   947.00    .0036    16.87     1.95      .63      .11     2.69      .13
   249   967.00    .0035    16.94     1.95      .63      .11     2.69      .14
   250   987.00    .0035    17.00     1.94      .64      .12     2.69      .16
   251  1007.00    .0034    17.05     1.94      .64      .12     2.69      .18
   252  1027.00    .0033    17.11     1.93      .65      .12     2.70      .19
   253  1047.00    .0032    17.16     1.93      .65      .13     2.70      .21
   254  1067.00    .0031    17.21     1.92      .65      .13     2.70      .23
   255  1087.00    .0030    17.26     1.92      .66      .13     2.70      .25
   256  1107.00    .0030    17.31     1.91      .66      .14     2.71      .27
```

Table 36 OILENS Model Output--Aqueous Contaminants

Purpose: A summary of the OILENS output for the chemical constituent of the hydrocarbon.

Column	Column Heading	Contents
1	Time	The time in days since the beginning of the simulation.
2	Species Radius	The effective radius for the constituent in meters.
3	NAPL Dissolution	The dissolution rate of the NAPL in kilograms per day.
4	Species Dissolution	The dissolution rate of the constituent in kilograms per day.
5	Species Dissolution	The cumulative mass of the constituent dissolved in kilograms.
6	Mass Degraded	The cumulative mass of the constituent degraded in kilograms.
7	Mass Remaining	The mass of the constituent remaining in the lens in kilograms.
8	Water Concentration	The water phase concentration in milligrams per liter of the constituent in contact with the ground water.
9	Percent Mass Balance Error	The calculated percent error in the constituent mass, based on the mass influx to the lens.

```
               **************************************************
               *    OILENS MODEL OUTPUT--AQUEOUS CONTAMINANTS   *
               **************************************************
               Benzene transport from 1500 gal gasoline spill
                1.15% benzene in gasoline
                sandy soil, properties from Carsel and Parrish

          SPECIES   OIL      SPECIES  SPECIES MASS     MASS      WATER    P.C.
  TIME    RADIUS    DISSOL.  DISSOL.  DISSOL. DEGRADED REMAINING CONC.    MASS
 (DAYS)    (M)    (KG/D)   (KG/D)    (KG)      (KG)      (KG)    (MG/L)  ERROR
==============================================================================

25.83        2.00 .525E-02 .551E-04      .00      .00      .00      .12    .00
25.96        2.03 .531E-02 .131E-02      .00      .00      .07     2.80    .00
26.12        2.06 .540E-02 .269E-02      .00      .00      .15     5.60    .00
26.29        2.09 .550E-02 .387E-02      .00      .00      .24     7.87    .00
26.40        2.10 .556E-02 .450E-02      .00      .00      .29     9.05    .00
26.52        2.13 .563E-02 .517E-02      .00      .00      .35    10.24    .00
26.65        2.15 .571E-02 .579E-02      .00      .00      .41    11.27    .00
26.79        2.17 .579E-02 .645E-02      .00      .00      .48    12.33    .00
26.96        2.20 .589E-02 .713E-02      .00      .00      .56    13.36    .00
27.15        2.24 .600E-02 .782E-02      .01      .00      .65    14.34    .00
27.36        2.27 .613E-02 .851E-02      .01      .00      .75    15.24    .00
27.58        2.31 .626E-02 .920E-02      .01      .00      .85    16.07    .00
27.81        2.34 .641E-02 .983E-02      .01      .00      .96    16.77    .00
28.06        2.39 .655E-02 .105E-01      .01      .00     1.07    17.44    .00
```

{Intermediate results omitted}

```
607.0       15.09 .102     .647E-02    20.53      .00      .50      .64    .00
627.0       15.22 .104     .585E-02    20.65      .00      .45      .57    .00
647.0       15.35 .105     .530E-02    20.76      .00      .40      .51    .00
667.0       15.47 .106     .483E-02    20.87      .00      .36      .46    .00
687.0       15.58 .108     .442E-02    20.96      .00      .33      .41    .00
707.0       15.69 .109     .406E-02    21.04      .00      .30      .38    .00
727.0       15.80 .110     .375E-02    21.12      .00      .27      .34    .00
747.0       15.90 .111     .347E-02    21.19      .00      .25      .31    .00
767.0       16.00 .112     .323E-02    21.26      .00      .23      .29    .00
787.0       16.09 .113     .302E-02    21.32      .00      .21      .27    .00
807.0       16.18 .114     .283E-02    21.38      .00      .20      .25    .00
827.0       16.26 .115     .267E-02    21.44      .00      .19      .23    .00
847.0       16.34 .116     .252E-02    21.49      .00      .17      .22    .00
867.0       16.42 .117     .238E-02    21.54      .00      .16      .21    .00
887.0       16.49 .118     .226E-02    21.58      .00      .15      .19    .00
907.0       16.56 .119     .216E-02    21.63      .00      .15      .18    .00
927.0       16.63 .120     .206E-02    21.67      .00      .14      .17    .00
947.0       16.69 .120     .197E-02    21.71      .00      .13      .17    .00
967.0       16.76 .121     .189E-02    21.75      .00      .13      .16    .00
987.0       16.82 .122     .181E-02    21.79      .00      .12      .15    .00
1007.       16.88 .122     .175E-02    21.82      .00      .11      .14    .00
1027.       16.93 .123     .168E-02    21.86      .00      .11      .14    .00
1047.       16.98 .124     .163E-02    21.89      .00      .11      .13    .00
1067.       17.04 .124     .157E-02    21.92      .00      .10      .13    .00
1087.       17.09 .125     .152E-02    21.95      .00      .10      .12    .00
1107.       17.13 .125     .148E-02    21.98      .00      .09      .12     .0
```

Table 37 Saturation and Concentration Profile		
Purpose: A summary of the saturations and concentrations in the vadose zone.		
Column	Column Heading	Contents
1	Depth	The depth in meters.
2	Saturation	The NAPL phase saturation.
3	Concentration (water)	The dissolved constituent concentration in the water phase in milligrams per liter.
4	Dissolved NAPL Concentration	The dissolved NAPL concentration in the water phase in milligrams per liter.

NOTE: After an NAPL lens forms this profile is truncated at the top of the NAPL lens. A radial profile of the NAPL lens is then produced.

```
SATURATION AND CONCENTRATION PROFILE AT    25.0000
**************************************************
Benzene transport from 1500 gal gasoline spill
 1.15% benzene in gasoline
 sandy soil, properties from Carsel and Parrish


        DEPTH          SAT.  CONC.(WATER) DISSOL. NAPL CONC
     =====================================================
          .0000         .0500     .0000   10.0000
          .0000         .0500     .0000   10.0000
          .0001         .0500     .0000   10.0000
          .0006         .0500     .0000   10.0000
          .0014         .0500     .0000   10.0000
          .0024         .0501     .0000   10.0000
          .0034         .0501     .0000   10.0000
          .0042         .0501     .0000   10.0000
          .0047         .0501     .0000   10.0000
          .0049         .0501     .0000   10.0000
          .0049         .0501   26.3920   10.0000
          .0898         .0524   26.3920   10.0000
          .4360         .0618   26.3920   10.0000
          .9960         .0725   26.3920   10.0000
         1.6731         .0814   26.3920   10.0000
         2.3501         .0885   26.3920   10.0000
         2.9101         .0936   26.3920   10.0000
         3.2563         .0965   26.3920   10.0000
         3.3412         .0972   26.3920   10.0000
         3.3412         .0972   26.3920   10.0000
         3.4263         .0978   26.3920   10.0000
         3.7730         .1005   26.3920   10.0000
         4.3338         .1044   26.3920   10.0000
         5.0119         .1089   26.3920   10.0000
         5.6899         .1130   26.3920   10.0000
         6.2507         .1162   26.3920   10.0000
```

```
          6.5975          .1181   26.3920   10.0000
          6.6825          .1186   26.3920   10.0000
          6.6825          .1186   26.3920   10.0000
          6.7646          .1190   26.3920   10.0000
          7.0995          .1208   26.3920   10.0000
          7.6411          .1235   26.3920   10.0000
          8.2959          .1267   26.3920   10.0000
          8.9507          .1296   26.3920   10.0000
          9.4923          .1320   26.3920   10.0000
          9.8272          .1335   26.3920   10.0000
          9.9093          .1338   26.3920   10.0000
          9.9093          .1338     .0000   10.0000
          9.9114          .1338     .0000   10.0000
          9.9196          .1338     .0000   10.0000
          9.9330          .1339     .0000   10.0000
          9.9492          .1340     .0000   10.0000
          9.9654          .1340     .0000   10.0000
          9.9787          .1341     .0000   10.0000
          9.9870          .1341     .0000   10.0000
          9.9890          .1341     .0000   10.0000


 KOPT PROFILE MASS PER UNIT AREA:
 NAPL                          (KG/M/M)  323.8
 DISSOLVED NAPL                (KG/M/M)  .2132E-01
 CONSTITUENT                   (KG/M/M)  3.708

 KOPT PROFILE TOTAL MASS:
 CONSTITUENT                       (KG)  46.60
 NAPL                              (KG)  4069.
```

Table 38 Radial Profile Through the NAPL Lens

Purpose: A radial description of the NAPL lens

Column	Column Heading	Contents
1	Radius	Radial distance in meters.
2	Current NAPL Lens--Depth of Top of Lens	The depth in meters from the ground surface to the top of the current NAPL lens.
3	Current NAPL Lens--Depth of Lens Bottom	The depth in meters from the ground surface to the bottom of the current NAPL lens.
4	Maximum Extent of NAPL Lens--Depth of Top of Lens	The depth in meters from the ground surface to the top of the thickest lens that has occurred previous to this time. The NAPL is trapped at the vadose zone residual between the depths for columns 2 and 4.
5	Maximum Extent of NAPL Lens--Depth of Top of Lens	The depth in meters from the ground surface to the bottom of the thickest lens that has occurred previous to this time. The NAPL is trapped at the aquifer residual between the depths for columns 3 and 5.

```
**************************************************
* RADIAL PROFILE THROUGH OIL LENS
**************************************************
TIME                 =    25.0000
LENS RADIUS          =     2.0213
DEPTH TO WATER TABLE =    10.0000

                    CURRENT OIL LENS          MAXIMUM EXTENT OF OIL LENS
  RADIUS         DEPTH OF        DEPTH OF        DEPTH OF        DEPTH OF
               TOP OF LENS     LENS BOTTOM     TOP OF LENS    LENSBOTTOM
==========     ===========     ===========     ===========  ===========

     .0000          9.9890         10.0025          9.9890        10.0025
    2.0000          9.9890         10.0025          9.9890        10.0025
    2.0011          9.9891         10.0024          9.9891        10.0024
    2.0021          9.9891         10.0023          9.9891        10.0023
    2.0032          9.9891         10.0023          9.9891        10.0023
    2.0043          9.9891         10.0022          9.9891        10.0022
    2.0053          9.9892         10.0021          9.9892        10.0021
    2.0064          9.9892         10.0021          9.9892        10.0021
    2.0075          9.9892         10.0020          9.9892        10.0020
    2.0085          9.9893         10.0019          9.9893        10.0019
    2.0096          9.9893         10.0018          9.9893        10.0018
    2.0107          9.9893         10.0017          9.9893        10.0017
    2.0117          9.9894         10.0017          9.9894        10.0017
    2.0128          9.9894         10.0016          9.9894        10.0016
    2.0139          9.9894         10.0015          9.9894        10.0015
    2.0149          9.9895         10.0014          9.9895        10.0014
    2.0160          9.9895         10.0012          9.9895        10.0012
    2.0171          9.9896         10.0011          9.9896        10.0011
    2.0181          9.9896         10.0010          9.9896        10.0010
    2.0192          9.9897         10.0008          9.9897        10.0008
    2.0203          9.9898         10.0006          9.9898        10.0006
    2.0213          9.9900         10.0000          9.9900        10.0000

     CUMULATIVE INFLUX TO LENS  17.35


     KOPT AND OILENS GLOBAL MASS BALANCES
     TOTAL NAPL MASS ADDED AT BOUNDARY  (KG)  4091.
     NAPL MASS RECOVERED BY MASS BALANCE (KG) 4086.
     PER CENT ERROR                          -.1285
```

6.2 HSSM-T Output File

The HSSM-T output file contains the items shown in Table 39.

Table 39 HSSM-T Output File Summary

Table Title	Contents
Input Data	Echo printing of the input parameter values.
Reduced Input Mass Flux	The mass flux history used by HSSM-T. The input mass flux is reduced to 31 values.
Aquifer Concentration History	Concentration histories for each receptor location.

```
Benzene transport from 1500 gal gasoline spill
 1.15% benzene in gasoline
 sandy soil, properties from Carsel and Parrish


 TSGPLUME

   INPUT DATA:
   ===========




   HSSM-KO INPUT DATA FILE   x2bt.dat
   HSSM-KO OUTPUT FILE         x2bt.HSS
   HSSM-T INPUT FILE           x2bt.PMI
   HSSM-T OUTPUT FILE          x2bt.TSG
   HSSM-T PLOT FILE            x2bt.PMP
   HSSM ENDING PARAMETER, KKSTOP          4
   INTERFACE FLAG                D

   LONG. DISPERSIVITY   = 10.00     (M)
   TRANS. DISPERSIVITY  = 1.000     (M)
   VERT. DISPERSIVITY   = .1000     (M)
   SEEPAGE VELOCITY     = .4128     (M/D)
   POROSITY             = .4300     (*)
   AQUIFER THICKNESS    = 15.00     (M)


   RETARDATION FACTOR   = 1.291     (*)
   P.C. MAX RADIUS      = 101.0     (*)
   MIN. AQUIFER CONC.   = .1000E-02 (MG/L)
   DECAY COEFFICIENT    = .0000     (1/D)


   BEGINNING TIME       = 100.0     (D)
   ENDING TIME          = 5000.     (D)
   TIME INCREMENT       = 50.00     (D)
```

```
   NO. OBS. WELLS       =       6   (*)

   X-LOCATION Y-LOCATION
   ---------- ----------
    25.00      .0000
    50.00      .0000
    75.00      .0000
    100.0      .0000
    125.0      .0000
    150.0      .0000

   RECHARGE RATE       =     .00 (M/D)
```

HSSM-KO is capable of producing very large output files, which if used directly in HSSM-T would cause HSSM-T to execute very slowly. HSSM-T extracts a reduced mass flux input history from the HSSM-KO output contained in file ***.PMI**. The reduced mass flux input always contains 31 points.

```
      REDUCED INPUT MASS FLUX
     HISTORY USED FOR COMPUTATION
     =============================

        TIME    MASS FLUX
        (D)      (KG/D)
     --------- ---------
   1  25.83      .5510E-04
   2  45.56      .3551E-01
   3  65.30      .5216E-01
   4  85.03      .6225E-01
   5  104.8      .6770E-01
   6  124.5      .6990E-01
   7  163.8      .6743E-01
   8  203.2      .6015E-01
   9  242.5      .5114E-01
  10  281.9      .4203E-01
  11  321.2      .3379E-01
  12  360.5      .2685E-01
  13  399.9      .2122E-01
  14  439.2      .1675E-01
  15  478.6      .1333E-01
  16  517.9      .1057E-01
  17  557.2      .8479E-02
  18  596.6      .6845E-02
  19  635.9      .5605E-02
  20  675.3      .4661E-02
  21  714.6      .3942E-02
  22  753.9      .3387E-02
  23  793.3      .2960E-02
  24  832.6      .2628E-02
  25  872.0      .2350E-02
  26  911.3      .2138E-02
  27  950.6      .1955E-02
  28  990.0      .1801E-02
  29  1029.      .1674E-02
  30  1069.      .1566E-02
  31  1108.      .0000
```

```
  TIME STEP TOO SMALL RELATIVE TO MASS FLUX DURATION
  MODIFIED TIME STEP       = 108.2     (D)
```

```
  MAXIMUM RADIUS           = 17.13     (M)
  MAX. RADIUS TIME          = 1107.     (D)
  RADIUS AT MAX. FLUX       = 8.510     (D)
  MAX. FLUX TIME            = 124.5     (D)
  EFFECTIVE RADIUS          = 8.510     (M)
  EFFECTIVE AREA            = 227.5     (M^2)
  PENETRATION THICKNESS     = 1.979     (M)
```

The HSSM-T results are written out as "aquifer concentration histories" for each of the receptor points. These consist of times and concentrations calculated for the receptor location.

```
AQUIFER CONCENTRATION HISTORIES
===============================

   TIME     RECEPTOR LOCATION
            ( X      25.00 )
            ( Y        .00 )
----------   ----------
 30.09        .1002E-02
 51.74        1.696
 73.38        5.004
 84.20        6.450
 96.65        7.876
 108.5        8.974
 119.7        9.813
 130.4        10.43
 140.5        10.86
 150.1        11.13
 159.7        11.30
 169.8        11.41
 172.4        11.43
 174.9        11.44
 175.7        11.44
 177.5        11.44
 179.0        11.44
 180.5        11.43
 182.7        11.43
 186.1        11.40
 191.5        11.35
 200.9        11.22
 217.7        10.90
 249.2        9.985
 311.5        7.751
 370.6        5.721
 426.8        4.175
 480.2        3.071
 530.9        2.290
```

```
579.1        1.744
624.8        1.358
668.3        1.085
709.6        .8893
748.9        .7480
786.2        .6436
821.6        .5656
855.2        .5060
887.2        .4586
917.5        .4216
946.4        .3916
973.8        .3665
999.8        .3454
1025.        .3278
1048.        .3128
1070.        .3000
1093.        .2590
1116.        .1526
1138.        .7703E-01
1159.        .4481E-01
1179.        .2868E-01
1198.        .1956E-01
1216.        .1398E-01
1233.        .1035E-01
1250.        .7888E-02
1265.        .6158E-02
1280.        .4906E-02
1294.        .3978E-02
1307.        .3276E-02
1320.        .2735E-02
1332.        .2312E-02
1343.        .1976E-02
1354.        .1706E-02
1364.        .1486E-02
1374.        .1306E-02
1383.        .1157E-02
1400.        .9268E-03
```

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Appendix 1 The MS-DOS Interface, HSSM-DOS

The DOS interface for HSSM is divided into the three major parts described below. All are independent programs that can be executed separately from the DOS prompt. For the convenience of the user, a simple menu program called HSSM-DOS can be used to run the programs in sequence. Each component of the DOS interface is described in detail in the following sections.

1.1 The HSSM-DOS Menu program

HSSM-DOS has six options for running the components of HSSM. Running the model generally follows the order of the menu options: creating and editing input data files with PRE-HSSM, running the simulations with HSSM-KO and HSSM-T, and plotting the results with HSSM-PLT.

Table 40 HSSM-DOS Menu

```
*********************************************
*              MENU FOR HSSM                *
*********************************************
1.     Prepare Input Data Files  RUN PRE-HSSM
2.     View Directory
3.     Run KOPT and OILENS       RUN HSSM-KO
4.     Run TSGPLUME              RUN HSSM-T
5.     Graph Results             RUN HSSM-PLT
6.     Exit
*********************************************
ENTER SELECTION (1-6):
```

The following sections introduce each portion of the DOS interface. Each of these descriptions contains references to the sections that contain detailed information on using the interface components.

1.2 Data Entry in PRE-HSSM

PRE-HSSM is a simple interactive preprocessor for the HSSM. PRE-HSSM allows the user to create data files by means of an interactive set of menus. The user has no need to know the structure of the data file. Several input data sets may be created within one session of PRE-HSSM and saved in disk files for future use by the HSSM. Also, data files created from earlier PRE-HSSM sessions may be read in and modified. The parameter names and a brief description of their use are displayed within each menu of the preprocessor. The data entry screens are discussed in detail in Appendix1.8. Although this information is provided on-line, it does not make the model self-explanatory. The user must refer to the user's guide for specific instructions on running the model. All data entered in PRE-HSSM must be written to a file before it is used by HSSM. Any data not saved before exiting PRE-HSSM or starting with a new data set will be lost. Minimal checking of parameter values is done in PRE-HSSM, so the user must assure that the values are reasonable.

1.3 Computation by HSSM-KO and HSSM-T

The two executables, HSSM-KO and HSSM-T, perform the HSSM simulations. HSSM-KO contains the KOPT and OILENS models and is run first. Using a previously created input data file, HSSM-KO creates a formal output file, several plot files and, if the appropriate flags and conditions are set, the input data file for HSSM-T. During execution, data is written into several temporary files. These files are concatenated upon successful execution into the output and plot files. The temporary files are then deleted from the hard disk. If HSSM-KO execution is interrupted, the temporary files remain on the hard disk. The program REBUILD can then be used to create as many of the output files as possible. The TSGPLUME module of HSSM is run by executing HSSM-T. This program also produces a formal output file and a plot file. Directions for use of the DOS commands for HSSM-KO and HSSM-T are given in Appendix 1.9.

1.4 Graphing of Results in HSSM-PLT

Although much useful information is contained within the HSSM-KO and HSSM-T formal output files, graphical display of the model results is also desirable and useful. HSSM-PLT allows the display and printing of HSSM output. The plot files which are automatically created by HSSM-KO and HSSM-T are used by HSSM-PLT to graph the output. Seven different types of graphs are avalable to the user. These graphs are displayed on the screen and may be printed on several types of printers and plotters. Specific information for using HSSM-PLT is given in appendix 1.10.

1.5 Quick Summary of the DOS Interface Commands

The following table lists the MS-DOS commands that can be used to run the HSSM without running the HSSM-DOS menu program. The full details of the procedures are described in the following sections.

Table 41 Quick Summary of MS-DOS HSSM Commands

Command	Action
For automated use of the interface:	
HSSM-DOS	Activates the DOS menu program which automatically executes the commands listed below.
For manual entry of commands at the DOS prompt:	
PRE-HSSM	Executes the interactive input data preprocessor.
HSSM-KO **name.DAT**	Executes the KOPT and OILENS modulates of HSSM, using the **name.DAT** data set.
HSSM-T **name.PMI**	Executes the TSGPLUME module of HSSM, using the **name.PMI** input data set generated by previous execution of HSSM-KO.
HSSM-PLT	Executes the interactive graphical post processor.

Note that HSSM requires a fixed set of file types for its input and output files. HSSM-T and HSSM-PLT only function properly when the required files types are used. PRE-HSSM can be used to generate the required file types automatically. The required files types are described in Table 15 of Section 4.7.

1.6 System Requirements

To use the DOS interface, the user should be generally familiar with personal computers, DOS, and the HSSM model. Also, users are assumed to be knowledgeable about their system hardware (i.e., which output device is connected to which port). The hardware and software requirements for using the MS-DOS interface are listed below.

☐ DOS 5.0 or higher
☐ 400 kilobytes of free RAM
☐ Hard drive (recommended)

Usage of the HSSM-PLT graphics package requires the following :

☐ Graphics device that is EGA, VGA, or better.
☐ ANSI.SYS driver installed in the CONFIG.SYS file.

The following printers are supported:

1) EPSON 9-pin, narrow carriage
2) EPSON 24-pin, LQ series, narrow carriage
3) EPSON 24-pin, LQ series, wide carriage
4) NEC Pinwriter, 24-pin, narrow carriage
5) NEC Pinwriter, 24-pin, wide carriage
6) Okidata, 9-pin, narrow carriage
7) HP LaserJet/DeskJet - low res.
8) HP LaserJet/DeskJet - medium res.
9) HP LaserJet/DeskJet - high res.
10) HP PaintJet - 2 color, low res.
11) HP PaintJet - 4 color, med res.
12) HP PaintJet - 8 color, high res.
13) HP PaintJet - 16 color, high res.
14) Postscript printer
15) HP - HPGL plotter
16) HP LaserJet III - HPGL/2 mode
17) Houston Instruments DM/PL plotter

The amount of available system memory may be checked by entering the DOS 5.0 `MEM` command. The amount of memory available for running a DOS program will be displayed. This amount must exceed 400 kbytes in order to run HSSM-KO. Although DOS 5.0 is stated as the minimum level of DOS required to run HSSM, earlier versions will likely be adequate; versions below 5.0 have not been tested.

1.7 Installation

The HSSM software is distributed on two high density diskettes. A backup copy of these diskettes should be made and subsequent work should be performed from the backup copies. The distribution diskette for HSSM-DOS (HSSM-1-d) contains the files indicated in Table 42.

Table 42 Packing List of Files for the HSSM-DOS Interface

File	Purpose
HSSM-DOS.EXE	The DOS menu program
PRE-HSSM.EXE	Interactive input data processor
HSSM-KO.EXE	The KOPT and OILENS modules of HSSM
HSSM-T.EXE	The TSGPLUME module of HSSM
HSSM-PLT.EXE	Interactive graphical postprocessor
REBUILD.EXE	A recovery program for interrupted simulations
CONFIG.PLT	Hardware configuration file for **HSSM-PLT.EXE**
SIMPLEX1.FNT	Font file for **HSSM-PLT.EXE**
README.TXT	Read me file containing distribution information
RAOULT.EXE	Utility to perform Raoult's Law Calculation
RAOULT.DAT	Default data set for the RAOULT utility
SOPROP.EXE	Utility to estimate soil properties with Rawls and Brakensiek's (1985) regression equations.
NTHICK.EXE	Utility to estimate NAPL thickness at the water table

The following describes how to install the model. Check the **README.TXT** file for information on automated installation procedures, as they are under development as of this writing. To create the HSSM directory enter the DOS command:

```
MKDIR C:\HSSM
```

where HSSM is the name of the HSSM-DOS subdirectory. With the HSSM-1-d diskette in drive A, copy all of the files from the diskette into the HSSM directory with the DOS command:

```
COPY A:\*.* C:\HSSM
```

(The program can be installed from another drive, say B, by replacing `"A:"` in the previous command with `"B:")`. The example problems and output files contained on diskette HSSM-2 should be installed into a separate directory. Create the example problem directory by entering:

```
MKDIR C:\HSSM\EXAMPLE
```

After putting the HSSM-2 diskette into drive A, the files are copied to this directory by entering:

```
COPY A:\*.* C:\HSSM\EXAMPLE
```

Subdirectories can and should be created for each HSSM simulation. For example, to create a directory PROJECT1, enter the command:

```
MKDIR C:\HSSM\PROJECT1
```

By issuing the DOS command

```
CD \HSSM\PROJECT1
```

before executing HSSM, all the input and output files for the simulation will be in `C:\HSSM\PROJECT1`. Installation of both the DOS and Windows interfaces on one machine is discussed in Appendix 9.

Once HSSM-DOS has been loaded onto your system, you must check the **CONFIG.SYS** file. The HSSM-KO program opens a number of temporary files and **CONFIG.SYS** must be configured so that a sufficient number of files may be opened. The **CONFIG.SYS** on your system needs to include the line

```
FILES = 30
```

(A number greater than 30 will also work.) To use HSSM from any directory add `C:\HSSM` to the path statement in your **AUTOEXEC.BAT** file. After modifying these files you must reboot your system to allow the change to take effect.

1.8 Using the PRE-HSSM Preprocessor

The first step in running HSSM is to run the preprocessor PRE-HSSM to create and/or edit input data sets. PRE-HSSM is provided as a convenience to the user; its usage greatly facilitates the generation of input data sets. For convenience, blank templates for each of these screens are provided in Appendix 12. These templates are useful for assembling data sets and may be copied for repeated usage. Appendix 10 shows the structure of the HSSM-KO and HSSM-T input data files for experienced users of HSSM who may wish to edit directly their input data sets.

Table 43 Introductory PRE-HSSM Screen

```
          ***************************************************
          *                                                 *
          *              PRE-HSSM VERSION 1.50              *
          *                                                 *
          *  AN INTERACTIVE PREPROCESSOR FOR THE HSSM MODEL *
          *                                                 *
          *                   JIM WEAVER                    *
          *  UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  *
          *   R.S. KERR ENVIRONMENTAL RESEARCH LABORATORY   *
          *                ADA, OKLAHOMA 74820              *
          *                  DONALD COLLINGS                *
          *       NSI TECHNOLOGY SERVICES CORPORATION       *
          *              ENVIRONMENTAL SCIENCES             *
          *                ADA, OKLAHOMA 74820              *
          *                   NOV 7, 1992                   *
          *                                                 *
          ***************************************************

DO YOU WANT TO READ AN EXISTING DATA FILE ?

  ENTER 0 OR <RETURN> IF NO
  ENTER 1             IF YES
  ENTER 2             TO VIEW DIRECTORY
  ENTER 3             FOR SAMPLE INPUT DATA SET
  ENTER 4             TO EXIT THE PREPROCESSOR
```

The main screen for the PRE-HSSM preprocessor is shown in Table 43. The screen also displays the file selection menu. The options available to the user are

0. Enter 0 or **<RETURN>** to create a new data set.

1. Enter 1 followed by **<RETURN>** to edit a previously created data set. The message

```
ENTER THE INPUT DATA FILE NAME
----+---*-40-character-limit*----+----*
```

is written to the screen. Forty characters are allowed for the data file name. A DOS path name can be included. If the file does not exist, the message

```
INPUT DATA FILE DOES NOT EXIST--REENTER
```

appears on the screen. If the file is not a valid HSSM input file, the message

```
INVALID INPUT DATA FILE
Stop - Program terminated.
```

appears and the program must be restarted.

2. Enter 2 followed by **<RETURN>** to view the current directory. This option executes the DOS command `DIR |MORE`, so that the directory is viewed one screen at time. After completing the command the user is returned to the file selection menu.

3. Enter 3 followed by **<RETURN>** to edit a sample data set. This data set is provided purely for the convenience of the user and is not intended for application to specific problems.

4. Exit the preprocessor by entering 4 and pressing <RETURN>.

1.8.1 Saving Data to a File

Before discussing the individual PRE-HSSM data menus, the procedure for saving data to files and exiting PRE-HSSM is explained. As previously noted, all data entered into PRE-HSSM must be written to a file before exiting or restarting PRE-HSSM, otherwise all entries and/or changes will be lost. The user is prompted for saving data before exiting or restarting.

Table 44 Writing Data Files

```
WRITE THE INPUT VALUES TO A FILE ?

*****************************************
***ANY DATA ENTERED IN PRE-KOPT MUST  ***
***BE WRITTEN TO A FILE BEFORE EXITING***
*****************************************

 ENTER 0 OR <RETURN> IF NO
 ENTER 1             IF YES
```

The screen shown in Table 44 prompts the user to decide whether or not to write the current data file to a disk file. This screen is displayed after the user has chosen no changes in the main menu (Table 47). To save the data to a disk file, enter 1; otherwise, press <RETURN>.

Table 45 Selecting File Names

```
CHOOSE A FILE TO WRITE TO:
CURRENT INPUT FILE NAME:  sample.dat
CURRENT OUTPUT FILE NAME:  <<NONE>>

 ENTER 0 OR <RETURN> TO EXIT WITHOUT WRITING TO ANY FILE
 ENTER 1             TO CHANGE THE DATA FILE NAME
 ENTER 2             TO OVERWRITE THE CURRENT INPUT FILE
```

When 1 is entered on Table 44, Table 45 appears, displaying the current input file name and the current output file name, and gives the user three options.

Enter 0 or **<RETURN>** to exit without writing any data file.

Enter 1 to change the name of the data file and write the data to that file.

Enter 2 to write the data to the current input file name.

Table 46 Exiting PRE-HSSM

```
DO YOU WANT TO CONTINUE ?


 ENTER 0 OR <RETURN> TO CONTINUE WITH THE SAME DATA SET
 ENTER 1             TO RESTART WITH A NEW DATA SET
 ENTER 2             TO EXIT THE PREPROCESSOR
```

After choosing whether or not to write a disk file, the user is prompted whether to continue PRE-HSSM or to exit (Table 46).

0. Enter 0 or **<RETURN>** to continue with the same data set that has just been created or edited. This option returns control to the PRE-HSSM Main Menu (Table 47).

1. Enter 1 and press **<RETURN>** to restart PRE-HSSM with a new data set. This option returns control to the Introductory PRE-HSSM Screen (Table 43).

2. Enter 2 and press **<RETURN>** to exit PRE-HSSM. By selecting this option the user is returned to the DOS prompt. Data previously written to files is retained on the disk; data not previously written to files is lost.

1.8.2 PRE-HSSM Main Menu Commands

Table 47 lists the names of the PRE-HSSM data entry screens. Most of the lines in the main menu correspond to one line in the data file used by the model. The following options are available for use with this menu and each of its sixteen sub-menus:

1. Enter 0 or press **<RETURN>** for no changes to any data item.

2. Select a line number to view/edit the data fields associated with it by entering a line number from 1 to 16 and pressing **<RETURN>**.

3. Enter -1 and press <**RETURN**> to view/edit all the sub-menus in sequence. This option will direct PRE-HSSM to go through each of the sub-menus. Once started, this option must be followed through to completion. There is no way to escape out of the sequence without losing all data entered during the session.

Table 47 PRE-HSSM Main Menu

```
         HSSM INPUT DATA SCREENS

         1......SIMULATION CONTROL SWITCHES
         2......OUTPUT AND PLOT FILE NAMES
         3......RUN TITLE
         4......MATRIX PROPERTIES
         5......HYDROLOGIC PROPERTIES
         6......HYDROCARBON (NAPL) PHASE PROPERTIES
         7......CAPILLARY SUCTION APPROXIMATION
         8......NAPL FLUX, VOLUME OR CONSTANT HEAD
         9......DISSOLVED CONSTITUENT CONCENTRATION
         10.....EQUILIBRIUM LINEAR PARTITION COEFFICIENTS
         11.....OILENS SUB-MODEL.1
         12.....OILENS SUB-MODEL.2
         13.....SIMULATION PARAMETERS
         14.....NUMBER OF PROFILES
         15.....PROFILE TIMES
         16.....TSGPLUME INPUT PARAMETERS

CHANGE OR VIEW INPUT DATA VALUES ?
 ENTER 0 OR <RETURN> FOR NO CHANGES
 ENTER <LINE NUMBER> FOR A SINGLE LINE
 ENTER -1            FOR ALL LINES IN SEQUENCE
```

1.8.3 Creating and Editing HSSM Data Sets

The following pages document each data entry menu. They are listed in the order they would appear if the user had chosen the -1 option on the PRE-HSSM main menu (review all items in the menu). The data items are grouped primarily by function within the model. As a result some parameters appear on screens to which, at first glance, they do not belong. This arrangement is due to the modularity of the code.

Each screen follows the following format: Each data item is numbered, and followed by its HSSM variable name is a short description of its use and its current value. To change a value, enter the item number and press **<RETURN>**, then enter the new value and press **<RETURN>** again. Each time a single modification or a series of modifications is completed, the preprocessor displays the new data for inspection and approval. Each data item may be modified any number of times while the screen is displayed, but only the values displayed just before the screen is exited are saved in main memory (RAM). After modifying all desired data items, the complete data set may be written to a disk file. Until this time all data is stored in RAM only, and will be lost if PRE-HSSM is exited or aborted.

The following units are used in HSSM and are listed with their usage and abbreviation. Care must be taken to assure that the inputs are converted to this set of units.

Table 48 Required Units for HSSM

Quantity	Unit	Abbreviation Used in PRE-HSSM
Time	day	D
Depth	meter	M
Dynamic viscosity	centipoise	CP
Density	grams/cubic centimeter	G/CC
Surface tension	dyne/centimeter	DYNE/CM
Concentration	milligrams/liter	MG/L
Soil-water partition coefficient	liters/kilogram	L/KG
Dispersivity	meters	M
Various	dimensionless	*

Table 49 Simulation Control Switches

```
SCREEN 1.  SIMULATION CONTROL SWITCHES

              1 IWR    PRINTING SWITCH
                       O NO  OUTPUT FILES PRODUCED
                       1 ALL OUTPUT FILES PRODUCED
              2 IKOPT  ECHO PRINT ONLY (IF IWR = 1)
                       0 READ AND ECHO PRINT DATA ONLY
                       1 RUN KOPT MODEL
              3 ICONC  DISSOLVED CONSTITUENT SWITCH
                       0 NO CONSTITUENT PRESENT
                       1 SIMULATE DISSOLVED CONSTITUENT
              4 ILENS  OILENS SWITCH
                       0 DO NOT RUN OILENS MODEL
                       1 RUN OILENS MODEL
              5 ITSGP  TSGPLUME SWITCH
                       0 DO NOT CREATE TSGPLUME MODEL INPUT FILE
                       1 CREATE TSGPLUME MODEL INPUT FILE



  ENTER 0 OR <RETURN> FOR NO CHANGE
  ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
  ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the integer printing switch (0 or 1). Entering 0 causes no output to be produced, so normally 1 will be entered for this variable.

2. Enter the integer KOPT/echo printing switch (0 or 1). Entering 0 will echo print the input data set without performing a simulation (if IWR is set to 1). Entering 1 will cause the program to read the data and run the KOPT module of HSSM. KOPT simulates the infiltration of the NAPL through the vadose zone. KOPT must be run in order to run OILENS or TSGPLUME.

3. Enter the dissolved constituent switch (0 or 1). Entering 0 simulates NAPL phase flow without a dissolved constituent. Entering 1 allows the simulation of a dissolved constituent within the NAPL phase. TSGPLUME requires a dissolved constituent.

4. Enter the integer OILENS switch (0 or 1). Entering 0 will prevent the OILENS model from running. Entering 1 will allow the OILENS model to run, if the NAPL reaches the water in sufficient quantity.

5. Enter the TSGPLUME data creation switch (0 or 1). Entering 0 will prevent HSSM-KO from creating the TSGPLUME (HSSM-T) input data set. Entering 1 will allow HSSM-KO to create an input data set for TSGPLUME, if there is a dissolved constituent which reaches the water table.

In order for HSSM-T and the HSSM-PLT post processor to function properly, a specified set of file types (the three-character extension to the file name following the period; i.e., name.TYP) is *required* to be used by HSSM-KO. The PRE-HSSM interface automatically assigns the required file names whenever a data set is saved to the disk.

Table 50   Run Title

```
SCREEN 3.  RUN TITLE

       1..  BENZENE TRANSPORT FROM 1500 GAL GASOLINE SPILL
       2..  1.15% BENZENE IN GASOLINE
       3..  SANDY SOIL, PROPERTIES FROM CARSEL AND PARISH


   ENTER 0 OR <RETURN> FOR NO CHANGE
   ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
   ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

The Run Title Screen (Table 50) allows the user to enter three lines of up to 50 characters each of information related to the data set. A 50-character ruler bar is displayed for convenience when entering the title. The information from this screen is reproduced as headings throughout the output files generated by the KOPT/OILENS.

- Any one line may be modified by entering its number at the prompt, or
- All three lines may be modified in succession by entering -1 at the prompt.
- The current title is accepted by pressing <RETURN> or entering 0.

Table 51 Porous Medium Properties

```
    SCREEN 4.   MATRIX PROPERTIES

         1 WKS   SATURATED VERTICAL HYDRAULIC
                 CONDUCTIVITY (M/D)                 7.1000
         2 RKS   RATIO OF HORIZONTAL TO VERTICAL
                 CONDUCTIVITY (*)                   2.5000
         3 KRF   RELATIVE PERMEABILITY SELECTION         2
                 INDEX
                 1 = BURDINE--BROOKS/COREY
                 2 = BURDINE--EQUIVALENT VAN GENUCHTEN
         4 XLAMB PORE SIZE INDEX (*)                2.6800
                 IF KRF = 1,  LAMBDA
                 IF KRF = 2,  N
         5 ETA   POROSITY (*)                       0.4300
         6 SWR   RESIDUAL WATER SATURATION (*)      0.1000


     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the value of the saturated vertical water phase hydraulic conductivity, K_s, in meters per day. Saturated hydraulic conductivity is one of the most important parameters of the model. Estimation of this parameter is described in Appendix 3.1 "Soil Properties." This appendix contains data from two tabulations of soil properties.

2. Enter the ratio of the horizontal saturated water phase conductivity to the saturated vertical water phase hydraulic conductivity. Anisotropy is not treated directly in HSSM, rather the model uses the product of the ratio RKS and the saturated vertical conductivity, K_s, to determine the hydraulic conductivity of the aquifer. This latter conductivity is also used for determining the effective conductivity to the NAPL for the lens spreading. The relationships between the conductivities are summarized inTable 52.

Table 52 Summary of Hydraulic Conductivity Relationships

Model and Region	Hydraulic Conductivity Used	HSSM Variables
Vadose zone (KOPT)	Vertical	K_s
NAPL lens (OILENS)	Horizontal	K_s*RKS
Aquifer (TSGPLUME)	Horizontal	K_s*RKS

3. Select the capillary pressure model by entering 1 for Brooks and Corey or 2 for the equivalent van Genuchten.

Choose the capillary pressure model to be used in HSSM calculations. Further information on the selection of the model parameters is given in Appendix 3.1 "Soil Properties." Either Brooks and Corey or van Genuchten model parameters may be used. The appendix contains typical parameter values for each of these models. Although the HSSM is designed to use the Brooks and Corey model, van Genuchten model parameters may be entered as input. The van Genuchten model parameters are converted to approximately equivalent Brooks and Corey model parameters by a procedure developed by Lenhard et al. (1989).

For the Brooks and Corey Model:

The Brooks and Corey (1964) model equation which describes the relationship between saturation S_w and capillary head h_c is given by

$$\left(\frac{S_w - S_{wr}}{1 - S_{wr}}\right) = \left(\frac{h_{ce}}{h_c}\right)^{\lambda} \qquad \textbf{(20)}$$

where the residual water saturation, S_{wr}, the air entry head ,h_{ce}, and the pore size distribution index, λ, are fitting parameters.

Brooks & Corey's λ

The parameter λ is called the pore size distribution index, and is determined either by fitting the Brooks and Corey model to the water/air capillary pressure curve $P_c(S_w)$ by a procedure outlined by Brooks and Corey (1964) or by non-linear curve fitting (e.g., van Genuchten et al., 1991).

For the van Genuchten Model:

NOTE: selecting the van Genuchten model causes HSSM to calculate approximately equivalent Brooks and Corey model parameters as described in Appendix 4.

van Genuchten's model is defined by

$$\frac{\theta_w - \theta_{wr}}{\theta_m - \theta_{wr}} = \frac{1}{\left[1 + (\alpha\, h_c)^n\right]^m} \qquad \textbf{(21)}$$

where

θ_w = volumetric water content
h_c = capillary head with units of m
θ_{wr} = volumetric residual water content
θ_m = volumetric maximum water content
α = a parameter with units of m^{-1}
n = a parameter
m = a parameter (taken as a simple function of n)

For HSSM the reduced water content term (the left hand side of van Genuchten's model is taken to be equal to

$$\frac{S_w - S_{wr}}{1 - S_{wr}} \qquad \textbf{(22)}$$

where the maximum water saturation, θ_m, is assumed to equal the porosity. The parameters of van Genuchten's model can be fitted to measured data by using a fitting program like RETC (van Genuchten et al., 1991).

4. Enter either the Brooks and Corey λ or van Genuchten n, depending on the capillary pressure curve model selected.

5. Enter the porosity, η

6. Enter the residual water saturation, which is determined from the measured capillary pressure curve.

Table 53 Hydrologic Properties

```
    SCREEN 5.  HYDROLOGIC PROPERTIES

         1 WMU     DYNAMIC VISCOSITY OF WATER (CP)    1.0000
         2 WRHO    DENSITY OF WATER (G/CC)            1.0000
         3 IRT     RECHARGE INPUT TYPE                     1
                   1 = FLUX SPECIFIED
                   2 = SATURATION SPECIFIED
         4 QW/SWMAX CONSTANT WATER FLUX OR SAT.       0.0140
                   FLUX: (M/D)
                   SATURATION: (*)
         5 XMKRW   MAX. WATER RELATIVE PERMEABILITY
                   DURING INFILTRATION (*)            0.5000
         6 WTABLE  DEPTH TO WATER TABLE (M)          10.0000


     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the dynamic viscosity of water, μ_w, in centipoise (cp). At 20°C the viscosity of water is 1.0 cp.

2. Enter the density of water, ρ_w in g/cm^3. At 20°C density of pure water is 1 g/cm^3.

3. Enter the type of recharge condition desired. Recharge can be specified either by specifying a recharge rate or be specifying a vadose zone residual water saturation.

Enter 1 to select a recharge flux for the recharge input:
Enter 2 to select a vadose zone water saturation.

4. Enter the water flux, q_w, in m/d or the saturation, $S_{w(max)}$ (*), depending on the rainfall input type selected in item 3.

When annual recharge is chosen for the recharge input:

The value entered is the average annual recharge rate. For example, with an annual recharge rate of 10 cm/yr the value entered is:

$$2.74\,x\,10^{-4}\ \frac{m}{d} = 10\ \frac{cm}{yr}\left(\frac{m}{100\,cm}\right)\left(\frac{yr}{365\,d}\right) \tag{23}$$

HSSM-KO calculates the water saturation (fraction of the pore space that is filled with water) from the recharge rate. Large recharge rates may cause the available pore space to be completely filled with water, allowing no NAPL to infiltrate. If such conditions are encountered an error message is written to the screen.

When water saturation is chosen for the recharge input:

If 35% of the pore space is filled by water, then 0.35 is entered here. Using the other set of units: if the volumetric moisture content is 0.14 and the porosity is 0.40, then the equivalent saturation of 0.35 is entered here.

Typically the moisture content at or above the *field capacity* would be used here, after converting to saturation. The relationship between volumetric moisture content, θ_w, porosity, η, and saturation, S_w, is given by $\theta_w = \eta S_w$. From the saturation input, HSSM-KO calculates the associated water flux.

5. Enter the maximum water relative permeability during infiltration, $k_{rw(max)}$. Since air is normally trapped during infiltration, the effective hydraulic conductivity of the soil will be less than the saturated conductivity. The relationship between effective conductivity to water, K_{ew}, and saturated conductivity to water, K_{sw} is given by

$$K_{ew} = K_{sw} k_{rw} \qquad \textbf{(24)}$$

where k_{rw} is called the relative permeability to water. The relative permeability equals zero when the saturation is at or below residual, and equals one when the porous medium is completely saturated with water.

To account for trapping of the air phase, the maximum effective conductivity is restricted by the value set for $k_{rw(max)}$. Typical values range from 0.4 to 0.6 (Bouwer 1966); 0.5 is often used (e.g., Brakensiek et al., 1981). The maximum water saturation is then determined from the k_{rw} function that is used by HSSM. The remainder of the pore space is assumed to be filled with trapped air. The water saturation calculated from $k_{rw(max)}$ is then discarded, as only the trapped air saturation is used by the model.

5. Enter the depth to the water table from the release point in meters. The release point is usually at the ground surface.

Table 54 Hydrocarbon (NAPL) Phase Properties

```
SCREEN 6  NAPL PHASE PROPERTIES

        1 PMU   DYNAMIC VISCOSITY OF NAPL (CP)   0.4500
        2 PRHO  NAPL DENSITY (G/CC)              0.7200
        3 SPR   RESIDUAL OIL SATURATION (*)      0.0500
        4 IAT   APPLICATION TYPE                      1
                1 = FLUX SPECIFIED
                2 = VOLUME/AREA SPECIFIED
                3 = CONSTANT HEAD PONDING
                4 = VARIABLE PONDING AFTER
                    CONSTANT HEAD PERIOD

     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the NAPL phase viscosity, μ_o, in centipoise. Typical NAPL viscosities are given below in **(26)**.

2. Enter the NAPL phase density, ρ_o, in g/cm^3. For OILENS simulations, the NAPL density must be less than that of water. Densities greater than water may be used if no OILENS simulation is performed. Some typical NAPL densities are given below in Table 55.

Hydrocarbon densities are sometimes expressed by the degrees API (Perry and Chilton, 1973) scale adopted by the American Petroleum Institute. Degrees API is defined by

$$^{\circ}API = \frac{141.5}{sp.gr.} - 131.5 \tag{25}$$

where sp.gr. is the specific of the NAPL measured at 70° F divided by the specific gravity of water measured at 60° F. The degrees API scale runs from 0.0 to 100.0 and covers a range of specific gravities from 1.076 to 0.6112.

The densities and viscosities of the NAPL and water phases are used by HSSM-KO to estimate the saturated hydraulic conductivity to the NAPL phase, K_{so}, by

$$K_{so} = K_{sw} \frac{\mu_w}{\mu_o} \frac{\rho_o}{\rho_w} \tag{26}$$

where K_{sw} is the saturated hydraulic conductivity, μ_w and μ_o are the water and oil viscosities, and ρ_w and ρ_o are the respective densities.

Table 55 NAPL Densities and Viscosities at 20° C

Liquid	Density g/cm^3	Viscosity cp
Gasoline	0.75	0.45
Water	1.00	1.00
No. 2 Fuel Oil	0.87	5.9
Transmission Fluid	0.89	80

3. Enter the residual NAPL phase saturation for the vadose zone, S_{orv}. By definition, the NAPL phase does not flow at saturations less than or equal to residual. In this model, the residual NAPL saturation is assumed to be a known constant. Ideally, this would be obtained by measuring the NAPL/air capillary pressure curve in the presence of the amount of water filling a portion of the pore space. Treating the residual NAPL saturation as a constant is acknowledged to be an assumption, as in actuality the NAPL residual saturation may vary with the hydraulic gradient and with time as the NAPL weathers (Wilson and Conrad, 1984.) Typically the residual NAPL saturation in the vadose zone is less than that for the aquifer (with the same media properties). Typical hydrocarbon residual saturations vary from 0.10 to 0.20 in the vadose zone, and from 0.15 to 0.50 in the saturated zone (Mercer and Cohen, 1990). These values correspond more closely to "specific retention", as the term is used in ground water hydrology, rather than true residuals at large capillary pressure values. A different residual oil phase saturation for the saturated zone may be entered on the "NAPL Lens Sub-Model Parameters. 1" menu (Table 64, item 6).

4. Enter the NAPL phase boundary condition for the simulation. Four options are provided for specifying the way in which the NAPL enters the subsurface. Not all of the release parameters are needed for each release option; those necessary are noted on the data screens.

Release Options

① **Specified flux**

Specifies a constant flux of NAPL, corresponding to a known rate of application of NAPL to the ground surface for a specified time interval. Excess NAPL is assumed to run off at the surface.

② **Specified volume/area**

Specifies a volume per unit area of NAPL applied over a certain depth. This results in a fixed volume applied instantaneously, corresponding to a land treatment system or a landfill.

③ **Constant head ponding**

Specifies constant head ponding for a specified duration. The ponding depth abruptly goes to zero at the end of the release. This condition is used to simulate a hydrocarbon tank rupture which is contained within a berm, for example.

④ Variable ponding after a period of constant head ponding

Specifies constant head ponding for a specified duration, followed by a gradual decrease to zero head as the NAPL infiltrates.

The values of the necessary parameters are then entered in Table 58 , Table 59, Table 60, or Table 61.

Table 56 Capillary Suction Approximation Parameters

```
SCREEN 7.  CAPILLARY SUCTION APPROXIMATION PARAMETERS

        1 HWE    AIR ENTRY HEAD (M)                 4.5000
        2 WSIG   WATER SURFACE TENSION (DYNE/CM)   65.0000
        3 OSIG   NAPL SURFACE TENSION (DYNE/CM)    35.0000


    ENTER 0 OR <RETURN> FOR NO CHANGE
    ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
    ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. If the Brooks and Corey model has been selected, enter the absolute value of the air entry head, h_{ce}, in meters. This value is determined as a parameter from the water/air capillary pressure curve (see matrix properties, Table 51). If the van Genuchten model has been selected, enter α in meters^{-1}.

2. Enter the water/air surface tension, σ_{aw}, in dyne/cm. At 20°C the surface tension of pure water is 72.8 dyne/cm. A lower value, say 65 dyne/cm, may be appropriate for soils and/or contaminated sites.

3. Enter the NAPL/air surface tension, σ_{oa}, in dyne/cm. Table 57 shows typical surface tension values for several petroleum products.

Table 57 Surface Tensions of Several Fuels (Wu and Hottel, 1991)

Liquid	Surface tension (dyne/cm)
gasoline	26
kerosene	25-30
gas oil	25-30
lubricating fractions	34
fuel oils	29-32

Table 58 Hydrocarbon (NAPL) Flux Boundary Condition

```
   SCREEN 8A.  NAPL FLUX BOUNDARY CONDITION

         1 QP   NAPL FLUX (M/D)                    0.4522
         2 TPB  NAPL EVENT BEGINNING TIME (D)      0.0000
         3 TPE  NAPL EVENT ENDING TIME (D)         1.0000

     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the constant NAPL flux, q_o, in meters per day. NAPL phase fluxes in excess of the maximum effective NAPL phase conductivity are assumed to run off.

2. Enter the beginning time of the NAPL release in days, usually this is zero.

3. Enter the ending time of the NAPL release in days.

Table 59 Hydrocarbon (NAPL) Volume Per Unit Area Boundary Condition

```
  SCREEN 8B.  NAPL VOLUME/AREA BOUNDARY CONDITION

         1 PVOL NAPL VOLUME/AREA (M)              0.4000
         2 DPL  LOWER DEPTH OF NAPL ZONE   (M)    0.5000

     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the volume of the NAPL phase per unit surface area that is either placed in a land treatment facility or a landfill (cubic meters/square meter).

2. Enter the depth of the bottom of the contaminated zone, d_{pl} (meters).

Table 60 Hydrocarbon (NAPL) Constant Head Ponding Boundary Condition

```
SCREEN 8C.  CONSTANT NAPL HEAD BOUNDARY CONDITION

        1 TPB  NAPL EVENT BEGINNING TIME (D)      0.0000
        2 TPE  NAPL EVENT ENDING TIME (D)         1.0000
        3 HS   CONSTANT HEAD FOR IAT = 3 (M)      0.2000

    ENTER 0 OR <RETURN> FOR NO CHANGE
    ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
    ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the beginning time of the NAPL release in days, usually this is zero.

2. Enter the ending time of the NAPL release in days.

3. Enter the depth of constant head ponding, H_s, in meters.

Table 61 Hydrocarbon (NAPL) Variable Head Ponding Boundary Condition

```
  SCREEN 8D.  VARIABLE HEAD PONDING BOUNDARY CONDITION

        1 TPB  NAPL EVENT BEGINNING TIME (D)     0.0000
        2 TPE  END OF CONSTANT HEAD PERIOD (D)   1.0000
        3 HS   CONSTANT HEAD FOR TPB TO TPE (M)  0.2000

    ENTER 0 OR <RETURN> FOR NO CHANGE
    ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
    ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the beginning time of the NAPL release in days, usually this is zero.

2. Enter the ending time of the NAPL release in days.

3. Enter the depth of constant head ponding, H_s, in meters.

Table 62 Dissolved Constituent Concentration

```
SCREEN 9.  DISSOLVED CONSTITUENT CONCENTRATION

     1 COINI   INITIAL CONCENTRATION IN NAPL (MG/L) 8208.0000

  ENTER 0 OR <RETURN> FOR NO CHANGE
  ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
  ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the initial concentration of the chemical constituent in the NAPL phase, $c_{b(ini)}$, in mg/L. HSSM idealizes the multiphase/multicomponent system as consisting of an "NAPL" phase that contains some small fraction of a dissolved constituent. The dissolved constituent can partition between the fluids and the solid. The concentration in the NAPL of the chemical is entered here. For example benzene composes 1.14% by mass of the idealized gasoline mixture used by Baehr & Corapcioglu (1987). The initial benzene (the dissolved constituent) concentration in gasoline (the NAPL or "oil") is given by

$$C_b = f_b \, \rho_g \tag{27}$$

where C_b is the concentration of benzene in the gasoline, f_b, is the mass fraction of benzene in gasoline, ρ_g is the density of the gasoline. Therefore

$$C_b \, (g/cm^3) = \frac{1.14\%}{100} \, (0.73 \, g/cm^3) = 0.0083 \, g/cm^3 \tag{28}$$

Converting the gasoline concentration to the required units gives

$$C_b \, (mg/L) = C_b \, (g/cm^3) \left(\frac{1000 \;\; cm^3}{L} \right) \left(\frac{1000 \;\; mg}{g} \right) = 8300 \, mg/L \tag{29}$$

Table 63 Equilibrium Linear Partition Coefficients

```
  SCREEN 10.  EQUILIBRIUM LINEAR PARTITION COEFFICIENTS

        1 XXKO  NAPL/WATER (*)                      311.0000
        2 XXKS  SOLID/WATER  (L/KG)                   0.8300
        3 XXKSH SOLID/WATER (HYDROCARBON) (L/KG)      0.8300
        4 RHOS  BULK DENSITY (GR/CC)                  1.5100


     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the linear equilibrium partitioning coefficient between the NAPL and the water phase concentrations of the chemical constituent. By definition

$$c_o = K_o \, c_w \qquad \textbf{(30)}$$

where K_o is the dimensionless partition coefficient between the NAPL phase (c_o) and water phase (c_w) concentrations of the chemical constituent. The partitioning between the NAPL phase and the water phase depends on the composition of the NAPL. Estimation of K_o is discussed in Appendix 3.2 "NAPL/Water Partition Coefficient." A utility program for performing the necessary calculations, called RAOULT, is described in Appendix 6.

2. Enter the linear equilibrium partitioning coefficient, K_d, in liters per kilogram between the soil and the water phase concentrations (c_s and c_w) of the constituent. By definition

$$c_s = K_d \, c_w \qquad \textbf{(31)}$$

where K_d is the partition coefficient in liters per kilogram between the solid (c_s) and water phase concentrations (c_w). K_d is commonly estimated from the fraction organic carbon of the media, f_{oc}, and the organic carbon partition coefficient, K_{oc} as

$$K_d = f_{oc} \, K_{oc} \qquad \textbf{(32)}$$

(44)(44) in Appendix 3 lists K_{oc} values for several hydrocarbon constituents.

3. Enter the linear equilibrium partitioning coefficient between the soil and the water phase concentrations (c_s and c_w) of the hydrocarbon phase. Like the solubility of the NAPL phase, discussed below, this parameter is not critical. This coefficient is used for estimating the partitioning of the dissolved fractions of the NAPL (i.e., all of the NAPL chemicals except the chemical constituent of interest).

4. Enter the bulk density, ρ_b, of the soil in g/cm^3. Porosity, η, and bulk density, ρ_b are related by

$$\rho_b = \rho_s (1 - \eta) \tag{33}$$

where ρ_s is the solids density. The density of quartz is approximately 2.65 g/cm^3. The values for porosity and bulk density must be related by equation **(33)**.

Table 64 OILENS Model Parameters, First Screen

```
     SCREEN 11.  OILENS SUB-MODEL PARAMETERS.1

          1 RADI   RADIUS OF SOURCE  (M)                   2.0000
          2 RMF    RADIUS MULTIPLICATION FACTOR (*)        1.0010
          3 FRING  CAPILLARY THICKNESS PARAMETER (M)       0.0100
          4 VDISP  AQUIFER VERTICAL DISPERSIVITY (M)       0.1000
          5 GRAD   GROUNDWATER GRADIENT   (*)              0.0100
          6 SPRB   AQUIFER RESIDUAL NAPL SATURATION (*)    0.1500

      ENTER 0 OR <RETURN> FOR NO CHANGE
      ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
      ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the radius of the contaminant source, R_s, in meters. When no OILENS simulation is desired (Run OILENS is not selected on the Simulation Control Switches screen), a *per unit area* simulation can be performed by entering 0.5642 as the radius of the source. The resulting source area is 1.0 m^2.

2. Enter the value of the radius multiplication factor. A value of 1.001 is suggested for the radius multiplication factor (RMF). The RMF is used to multiply the source radius for starting the OILENS model. This is necessary since the OILENS equations are singular at the source radius. Starting the simulation at a small distance from the true radius avoids this singularity. This procedure does, however, introduce a mass balance error into the solution, so the minimum value of RMF which permits the simulation to proceed should be used. At no time should the RMF exceed 1.1. When the singularity is encountered, the OILENS model will display the error message

```
OILENS SINGULARITY ENCOUNTERED, INCREASE RMF
```

The RMF should then be increased and the simulation retried.

3. Enter the value of the capillary thickness parameter (meters). The capillary thickness parameter gives the model a thickness which must build up in the capillary fringe before spreading of the NAPL occurs. Typically, a value of 0.01m should be entered for this parameter. This results in a small thickness of NAPL that is built up before spreading begins.

The capillary thickness parameter can also be used to incorporate the effect of water table fluctuation on the lens radius. Water table fluctuation can cause trapping of NAPL throughout a smear zone, and the trapped NAPL is not available for radial spreading. To include this effect, the capillary thickness parameter should be calculated by

$$\begin{pmatrix} capillary \\ thickness \\ parameter \end{pmatrix} = \frac{smear\ zone\ thickness \times residual\ NAPL\ saturation}{maximum\ NAPL\ saturation\ in\ lens} \qquad \textbf{(34)}$$

The smear zone thickness should be taken as the maximum water table fluctuation. The residual NAPL saturation and maximum NAPL saturation in the lens are described under Screens 6, 11 and 12.

4. Enter the vertical dispersivity of the aquifer, A_V, in meters. See the discussion of longitudinal dispersivity under **(34)** below.

5. Enter the groundwater gradient. Typical maximum natural gradients are 0.005 to 0.02. Since pumping wells are not allowed in TSGPLUME, natural gradients should be used here.

6. Enter the residual NAPL phase saturation in the aquifer, S_{ors}. See notes above for vadose zone residual NAPL saturation.

Table 65 OILENS Model Parameters, Second Screen

```
    SCREEN 12.  OILENS SUB-MODEL PARAMETERS.2

       1 XMSOL    MAX. NAPL SATURATION IN LENS (*)         0.3260
       2 SOLC     CONSTITUENT WATER SOLUBILITY (MG/L)   1750.0000
       3 SOLH     HYDROCARBON WATER SOLUBILITY (MG/L)     10.0000

     ENTER 0 OR <RETURN> FOR NO CHANGE
     ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
     ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the saturation of the LNAPL, $S_{o(max)}$, in the NAPL lens. In HSSM, the lens is idealized as a uniformity saturated lens, although in actuality the NAPL saturation varies within the lens. The thickness of the lens in HSSM represents the ratio of the volume of the lens to its area. Within the lens the NAPL has a certain saturation. Estimation of the NAPL lens saturation is discussed in Appendix 3.3, and a utility called NTHICK for performing the necessary calculation is described in Appendix 7.

2. Enter the chemical constituent water solubility, s_k, in mg/L. The solubility entered here is the "pure component" solubility which is tabulated in several sources (i.e., Mercer et al., 1990; Sims et al., 1991; USEPA, 1990). Several values are given in Table 98. The solubility is used by HSSM to limit the water phase concentration. Appropriately chosen K_o values (which imply maximum water phase concentrations much less than the pure phase solubilities) make this parameter redundant for NAPLs composed of mixtures of chemicals.

3. Enter the NAPL water solubility in mg/L. This coefficient represents the solubility of all of the NAPL constituents, except the chemical constituent that is simulated. The solubility of the chemical constituent is entered separately. Further, this value is only used by the model in a substantial way if one of the ending criteria is used. Therefore the value of the NAPL solubility is not a critical parameter.

The value of NAPL solubility must be greater than zero if the **OILENS Simulation ending criterion** (see below) is set to ② "NAPL lens spreading stops." Bauman (1989) estimated that the typical solubility of gasoline is on the order of 50 to 200 mg/L.

Table 66 Simulation Control Parameters

```
SCREEN 13.  SIMULATION PARAMETERS

    1 TM     SIMULATION ENDING TIME  (D)          2500.0000
    2 DM     MAXIMUM SOLUTION TIME STEP  (D)        20.0000
    3 DTPR   MINIMUM TIME BETWEEN PRINTED TIME STEPS
             AND MASS BALANCE CHECKS (D)             0.1000
    4 KSTOP  ENDING CRITERION                             4
      1 = USER SPECIFIED TIME
      2 = LENS SPREADING STOPS
      3 = MAXIMUM CONTAMINANT MASS FLUX TO AQUIFER
      4 = CONTAMINANT MASS FLUX IN OILENS < OPERC * MAX
    5 OPERC  MINIMUM CONTAMINANT MASS IN LENS (*)    0.0100


ENTER 0 OR <RETURN> FOR NO CHANGE
ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the simulation ending time in days. This time must always be specified, even though other stopping options are available and may override the maximum simulation time.

2. Enter the maximum solution time step in days. This should be set as high as possible, although internal error correction routines will often limit the actual size of the step taken. Values of up to 25 days are usually acceptable. Overly large step sizes may introduce mass balance errors in the model results.

3. Enter the minimum time between printed time steps in days. Although the model uses a variable time step ordinary differential equation solver, at times during the simulation HSSM takes very small steps. Results from these steps are of little use and dramatically increase the size of the output files. This parameter prevents the output of every solution step and should be set to 0.1 or 0.25 days. This parameter does not affect the simulation itself, but only the information that is output.

For most chemicals leaching out of the lens, after the peak mass flux into the aquifer has passed, there is a relatively long period of time where the mass flux into the aquifer slowly declines. During this time period, the user set minimum time between printed time steps may be overridden in order to reduce the size of the output and plot files. An additional criteria is added that the mass flux must change by at least 1.0 percent for the results to be output. This feature cannot be overridden by the user.

4. The OILENS Simulation ending criterion determines how the HSSM-KO simulation terminates. Because it is not possible to predict when certain events in the simulation will occur, several of the options cause the simulation to end only after the event of interest has occurred. In these cases the user specified ending time is overridden and the simulation continues.

NOTE: The fourth option, "Contaminant leached from lens" must be chosen in order to use the HSSM-T model.

① User-specified ending time

Stop at the simulation ending time specified above.

② NAPL lens spreading stops

Stop the simulation when the NAPL lens stops spreading. If no NAPL lens forms before the specified ending time, then the simulation stops at the specified ending time. If a lens does form, the ending time is overridden and the simulation continues until the NAPL lens stops spreading. When the NAPL phase solubility is near zero, it is possible that, in the model, the lens motion may never stop, since kinematic theory predicts that an infinite amount of time is required for all of the NAPL to pass a given depth. The NAPL trickles into the lens throughout the simulation, and NAPL lens motion stops when the flux into the lens drops below the NAPL dissolution flux into the aquifer. If the NAPL solubility is zero and no chemical constituent is simulated, no NAPL is dissolved and the motion may continue indefinitely. To avoid this problem, *a non-zero NAPL solubility* (see Hydrocarbon Phase Parameters) is required for this situation.

③ Maximum contaminant mass flux into aquifer

Stop the simulation when the maximum chemical constituent flux into the aquifer occurs. If no NAPL lens forms before the specified ending time, the simulation stops at the specified ending time. If a lens forms, the ending time is overridden and the simulation continues until the maximum mass flux occurs.

④ Contaminant leached from lens drops below a given fraction of the total mass in the lens

Stop the simulation when the contaminant mass in the NAPL lens drops below a specified fraction of the maximum contaminant mass that has been contained within the lens during the entire simulation. The fraction is specified by the user. If no NAPL lens forms before the user-specified ending time (above), the simulation stops at the specified ending time.

5. Enter the mass factor stopping criterion for the ending criterion ④ "Contaminant leached from lens". Two percent (0.02) or less should be used for this factor.

Table 67 Number of Profiles

```
SCREEN 14.  PROFILES

     1 NTIMES  NUMBER OF PROFILES DESIRED (UP TO 10)         10

   ENTER 0 OR <RETURN> FOR NO CHANGE
   ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
   ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the number of KOPT saturation vs depth profiles (**Saturation Profiles** graph) and OILENS lens thickness vs. radius profiles (**NAPL Lens Profiles** graph). Both are produced at specified times (screen 15) along with mass balance approximations. Up to ten profiles are allowed.

Table 68   Profile Times

```
  SCREEN 15.  PROFILE TIMES

       PR ( 1) =     1.0000
       PR ( 2) =     2.0000
       PR ( 3) =     4.0000
       PR ( 4) =     5.0000
       PR ( 5) =     7.5000
       PR ( 6) =     9.0000
       PR ( 7) =   720.0000
       PR ( 8) =  1000.0000
       PR ( 9) =  1500.0000
       PR (10) =  2000.0000

   ENTER 0 OR <RETURN> FOR NO CHANGE
   ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
   ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

A maximum of ten profile times (days) may be entered depending on the value of NTIMES entered in screen 14.

Table 69 TSGPLUME Input Data Menu

```
        SCREEN 16.  TSGPLUME DATA INPUT SCREENS

                1......TSGPLUME INPUT DATA
                2......SIMULATION TIME
                3......WELL LOCATIONS

      ENTER 0 OR <RETURN> FOR NO CHANGE
      ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
      ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

From screen 16, three screens of TSGPLUME input data are assessed. None of these data are used in KOPT/OILENS for simulation, but are processed and printed in the TSGPLUME input data file. After the KOPT/OILENS simulation is completed the mass flux profile to the aquifer is added to the data file.

Table 70 TSGPLUME Data

```
      SCREEN 16A.  TSGPLUME DATA

          1 DLONG   AQUIFER LONGITUDINAL DISPERSIVITY (M)     10.0
          2 DTRAN   AQUIFER TRANSVERSE DISPERSIVITY (m)        1.0
          3 PMAX    PERCENT MAX. CONTAM. RADIUS (*)          101.0
          4 CMINW   MINIMUM OUTPUT CONCENTRATION (MG/L)      0.001
          5 ZLAM    AQUIFER DECAY RATE COEFFICIENT (1/D)       0.0
          6 NWELL   NUMBER OF RECEPTOR WELLS (*)                 2

      ENTER 0 OR <RETURN> FOR NO CHANGE
      ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
      ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the longitudinal dispersivity of the aquifer, A_L, in meters.

2. Enter the horizontal transverse dispersivity of the aquifer, A_T, in meters.

The dispersivities are defined by

$$\begin{aligned} D_L &= A_L\, v \\ D_T &= A_T\, v \\ D_V &= A_V\, v \end{aligned} \qquad \textbf{(35)}$$

where D_L, D_T, and D_V are the longitudinal, horizontal transverse, and vertical transverse dispersion coefficients; A_L, A_T, and A_V are likewise the longitudinal, horizontal transverse, and vertical transverse dispersivities; and v is the seepage velocity in the mean flow direction.

Dispersive mixing in aquifers results from solute transport through heterogeneous porous media. As the contaminant plume spreads it "experiences" more heterogeneity and the apparent dispersion coefficient increases. Thus the dispersion coefficients, D_L, D_T and D_V are not fundamental parameters, but exhibit scale dependence.

Gelhar et al. (1992) recently reviewed dispersivities determined at 59 sites and considered the reliability of the dispersion coefficients. They concluded that there are no highly reliable longitudinal dispersion coefficients at scales greater than 300m. Notably, at a given scale, dispersivities have been found to vary by 2 to 3 orders of magnitude, although the lower values are more reliable. Based on these data, horizontal transverse dispersivities are typically from 1/3 to almost 3 orders-of-magnitude lower than longitudinal dispersivities. Vertical transverse dispersivities are typically (although based on a very limited data set) 1-2 orders-of-magnitude lower than horizontal transverse dispersivities. The very low values of vertical transverse dispersivities reflect roughly horizontal stratification of sedimentary materials.

3. Enter the percentage of the maximum contaminant radius which is to be used in the TSGPLUME simulation, which requires a constant radius for the input mass flux.

Since the radius of the NAPL lens changes continuously during part of the simulation, it may not be possible to preselect an appropriate lens radius for the TSGPLUME module. It is desirable, however, to match the radius of the lens to the peak mass flux into the aquifer. Thus TSGPLUME simulation can use the radius which occurs at the time of the maximum mass flux. With this approach the peak mass flux is not overly diluted due to a large lens radius. (Nor is it "condensed" due to an overly small radius). The lens radius which occurs at the time of the maximum mass flux is automatically selected if 101 is entered for the percent maximum contaminant radius. Thus, the recommended value of this parameter is 101. It may be desirable for users to determine the effect of varying the size of the source on the aquifer concentrations.

4. Enter the minimum concentration (mg/L) for TSGPLUME to include in the output. Concentrations below this value will be reported as zero. A nonzero value of this parameter is required for proper execution of the TSGPLUME module. Typically, a concentration of 0.001 mg/L is suitable for the minimum concentration.

5. Enter the half-life of the constituent in the aquifer. This value is used only by the TSGPLUME model.

6. Enter the number of wells (a maximum of six) for which TSGPLUME is to calculate concentration vs time for the **Well Concentrations** graph.

Table 71 TSGPLUME Simulation Time

```
SCREEN 16B.  TSGPLUME SIMULATION TIMES

     1 BEGT    BEGINNING TIME (D)                    100.0
     2 ENDT    ENDING TIME (D)                      5000.0
     3 TINC    TIME INCREMENT (D)                     50.0
     4 TAQU    AQUIFER THICKNESS (M)                  15.0

ENTER 0 OR <RETURN> FOR NO CHANGE
ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

1. Enter the beginning time in days for the TSGPLUME simulation. See note below.

2. Enter the ending time in days for the TSGPLUME simulation. See note below.

3. Enter the time increment in days for TSGPLUME output between the beginning and ending times specified above. Typically 50 or 100 days is adequate for the time increment. See note below.

NOTE: Before running the model, it is not possible to guess precisely when the contaminant arrives at or passes a given receptor point. HSSM-T will override the user supplied beginning and ending times which allows the model to produce smooth concentration histories at the receptor point. Particular effort is expended in HSSM-T to calculate when the contaminant first arrives at the receptor point and when the peak concentration arrives. The duration of mass flux into the aquifer is used to determine a proposed time increment for HSSM-T output. If one hundredth of the mass flux input duration is greater than the user specified time increment the user is prompted to increase the time increment:

```
*** TSGPLUME RECOMMENDS CHANGING THE TIME INCREMENT
*** FROM  0.5000 DAYS TO 98.60 DAYS
*** ACCEPT THE CHANGE ? (Y OR N)
```

HSSM-T is making the user an offer that shouldn't be refused, at least for an initial simulation. If the resulting concentration history curve is not smooth enough, the user may reduce the time increment for HSSM-T to produce a finer spacing in time.

If the user does not accept the change, he/she is prompted to decide between the original time increment or to enter a new time increment.

4. Enter the thickness of the aquifer in meters.

Table 72 TSGPLUME Well Locations

```
SCREEN 16C.  WELL LOCATIONS

    #       X          Y
  ===== ========== ==========
    1       25.       00.
    2       50.       00.

  ENTER 0 OR <RETURN> FOR NO CHANGE
  ENTER <ITEM NUMBER> TO CHANGE SINGLE ITEM
  ENTER -1            TO CHANGE ALL ITEMS IN SEQUENCE
```

Enter up to six well locations, as X and Y coordinates in meters. X is directed along the longitudinal axis of the plume (the direction of groundwater flow) and Y is directed transversely distance to the X axis. The origin of the coordinate system is located at the center of the source (see **Figure 9**). The number of entries will be truncated depending on the value of **Number of receptor wells** on Table 70.

1.9 Running the KOPT, OILENS and TSGPLUME Modules

This section describes the operation of the HSSM-KO and HSSM-T modules. These programs are the heart of the simulation model. The DOS interface program (HSSM-DOS) can run the modules by shelling out to DOS and issuing the commands listed below. The HSSM-DOS commands are listed in Table 40. The user may also execute the commands directly from the DOS prompt.

Once an input data file has been created, the HSSM-KO module is executed by the DOS command

```
HSSM-KO NAME.DAT
```

where `NAME.DAT` is the input data file. The command assumes the default directory contains the HSSM-KO.EXE file, or that the HSSM directory has been added to the path (see Appendix 1.7). Table 73 shows the first screen that appears when HSSM-KO is executed. This screen identifies the model and the authors. Pressing return displays the disclaimer screen (Table 74). Carefully note the disclaimer messages. Sound scientific and engineering judgement is required when applying models and the user is responsible for the application of the model.

Table 73 Introductory HSSM-KO Screen

```
***************************************************
*                                                 *
*                    HSSM                         *
*                                                 *
*        HYDROCARBON SPILL SCREENING MODEL        *
*                                                 *
*  INCLUDING THE KOPT, OILENS AND TSGPLUME MODELS *
*                                                 *
*               JAMES W. WEAVER                   *
*  UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  *
*   R.S. KERR ENVIRONMENTAL RESEARCH LABORATORY   *
*             ADA, OKLAHOMA 74820                 *
*                                                 *
*  INCLUDING OILENS--HYDROCARBON MOVEMENT ON THE  *
*                 WATER TABLE                     *
*  RANDALL CHARBENEAU, SUSAN SHULTZ, MIKE JOHNSON *
*   ENVIRONMENTAL AND WATER RESOURCES ENGINEERING *
*       THE UNIVERSITY OF TEXAS AT AUSTIN         *
*                                                 *
*                 VERSION 1.00                    *
***************************************************
```

Table 74 Disclaimer Screen

```
***************************************************
 *                     WARNING:                     *
 * THIS PROGRAM SIMULATES IDEALIZED BEHAVIOR OF    *
 * OILY-PHASE CONTAMINANTS IN IDEALIZED POROUS     *
 * MEDIA, AND IS NOT INTENDED FOR APPLICATION TO   *
 * HETEROGENEOUS SITES.                            *
 * THE MODEL RESULTS HAVE NOT BEEN VERIFIED BY     *
 * EITHER LAB OR FIELD STUDIES.                    *
 * READ USER GUIDE FOR FURTHER INFORMATION BEFORE  *
 * ATTEMPTING TO USE THIS PROGRAM.                 *
 * NEITHER THE AUTHORS, THE UNIVERSITY OF TEXAS,   *
 * NOR THE UNITED STATES GOVERNMENT ACCEPTS ANY    *
 * LIABILITY RESULTING FROM THE USAGE OF THE CODE  *
 * THE U.S. E.P.A DOES NOT OFFICIALLY ENDORSE THE  *
 * USE OF THIS CODE.                               *
 ***************************************************
```

A list of the file names used by HSSM-KO and HSSM-T is displayed in Table 75.

Table 75 Output File Names and Run Options

```
OUTPUT AND PLOT FILE NAMES:

HSSM-KO INPUT DATA FILE    BENZENE.DAT
HSSM-KO OUTPUT             BENZENE.HSS
HSSM-KO PLOT 1             BENZENE.PL1
HSSM-KO PLOT 2             BENZENE.PL2
HSSM-KO PLOT 3             BENZENE.PL3
HSSM-T INPUT DATA FILE     BENZENE.PMI
HSSM-T OUTPUT              BENZENE.TSG
HSSM-T PLOT                BENZENE.PMP

TO RUN HSSM-KO          ENTER <RETURN>
TO CHANGE INPUT FILE    ENTER F
TO VIEW DIRECTORY       ENTER D
TO EXIT                 ENTER 1
```

The names must follow a strict naming convention for the TSGPLUME module (HSSM-T) and the HSSM-PLT post-processor to function properly. For the user's convenience the correct file names are generated automatically by PRE-HSSM. These should not be modified by the user.

As indicated in Table 75, the user may either run HSSM-KO, change the input data file, view the current directory or exit the program. Upon beginning a simulation the model writes messages to the screen as the computations proceed. These allow the simulation to be tracked by the user. Table 76 contains a typical set of screen messages for a simulation.

Table 76 Typical HSSM-KO Screen Messages

```
*** DATA INPUT
*** DATA INITIALIZATION
*** SIMULATION BEGINNING
*** OIL INFILTRATION
*** OIL REDISTRIBUTION
*** CHEMICAL REACHES WATER TABLE
*** OIL LENS FORMS
*** PROFILING AT      15.00 DAYS
*** PROFILING AT      30.00 DAYS
*** PROFILING AT      90.00 DAYS
*** PROFILING AT     130.00 DAYS
*** PROFILING AT     175.00 DAYS
*** SIMULATION END
*** POST PROCESSING
*** CREATING OUTPUT FILE:
*** BENZENE.HSS
*** PROCESSING PLOT FILE CONTENTS
*** REPACKING FILE 18
*** REPACKING FILE 19
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL1
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL2
*** CREATING KOPT/OILENS PLOT FILE:
*** BENZENE.PL3
*** CREATING TSGPLUME DATA FILE:
*** BENZENE.PMI
*** HSSM END
```

The HSSM-T implementation of TSGPLUME is designed to be used with HSSM-KO. If the data set for HSSM-KO has switches set appropriately, and if the dissolved chemical of interest reaches the water table (either through the formation of a NAPL lens or by the leaching from an immobilized NAPL body in the vadose zone), then an input data set for TSGPLUME is created by running HSSM-KO. The necessary flags and conditions for TSGPLUME data file generation are summarized in Table 77. These parameters are described in detail in Appendix 1.8.2.

Table 77 HSSM-KO Data Switches for the Creation of TSGPLUME (HSSM-T) input Data Files

Condition or switch	PRE-HSSM Screen	Effect
IWR = 1	Screen 1 (Table 49)	Output and plot files produced
IKOPT = 1	Screen 1 (Table 49)	KOPT module is run
ILENS = 1	Screen 1 (Table 49)	OILENS module is run
ICONC = 1	Screen 1 (Table 49)	Chemical constituent is included in the simulation.
ITSGP = 1	Screen 1 Table 49)	Attempt to create the TSGPLUME (HSSM-T.EXE) input data.
KSTOP = 4	Screen 13 (Table 66)	End HSSM-KO.EXE simulation when a small fraction of chemical constituent remains in the oil lens.
"large" simulation ending time (TM)	Screen 13 (Table 66)	Allow sufficient simulation time for chemical to reach the water table before ending simulation (with KSTOP = 4 simulation ending time is over-ridden if the chemical reaches the water table.)

Once HSSM-KO has run and produced an HSSM-T input data file, HSSM-T can be executed by entering the command:

```
HSSM-T NAME.PMI
```

where **NAME.PMI** is the input data file. When HSSM-T executes, screen messages appear as shown in Table 78. After pressing return, the file names for the simulation appear as indicated in Table 79.

Table 78 Introductory HSSM-T Screen

```
***************************************************
*                                                 *
*                   TSGPLUME                      *
*                                                 *
*      TRANSIENT SOURCE GAUSSIAN PLUME MODEL      *
*                                                 *
*                                                 *
*                  MIKE JOHNSON                   *
*               RANDALL CHARBENEAU                *
*        THE UNIVERSITY OF TEXAS AT AUSTIN        *
*                                                 *
*                   JIM WEAVER                    *
* ROBERT S. KERR ENVIRONMENTAL RESEARCH LABORATORY*
*  UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  *
*                                                 *
*                VERSION 1.00                     *
***************************************************
```

Table 79 HSSM-T Output File Names and Run Options

```
OUTPUT AND PLOT FILE NAMES:

HSSM-KO INPUT DATA FILE  BENZENE.DAT
HSSM-KO OUTPUT           BENZENE.HSS
HSSM-T INPUT             BENZENE.PMI
HSSM-T OUTPUT            BENZENE.TSG
HSSM-T PLOT              BENZENE.PMP

TO RUN TSGPLUME          ENTER <RETURN>
TO CHANGE INPUT FILE     ENTER F
TO VIEW DIRECTORY        ENTER D
TO EXIT                  ENTER 1
```

When HSSM-T executes, a set of messages is written to the screen (Table 80). These messages inform the user on the progress of the simulation. The example shown has only one receptor location; when more receptors are used, more messages like these are produced.

Table 80 Typical HSSM-T Screen Messages

```
  *** DATA INPUT
  *** DATA INITIALIZATION
  *** CALCULATING FLOATING POINT PRECISION
  ***
  *** COMPUTATION BEGINNING FOR RECEPTOR     1
  *** CALCULATING THE TOE TIME OF THE HISTORY
  *** SEARCH ALGORITHM COMPLETED IN    6 ITERATIONS
  *** COMPUTATION AT  18.18     DAYS COMPLETED
  *** COMPUTATION AT  18.44     DAYS COMPLETED
  *** COMPUTATION AT  33.41     DAYS COMPLETED
  *** COMPUTATION AT  48.38     DAYS COMPLETED
  *** COMPUTATION AT  63.35     DAYS COMPLETED
  *** COMPUTATION AT  78.32     DAYS COMPLETED
  *** COMPUTATION AT  83.32     DAYS COMPLETED
  *** COMPUTATION AT  88.32     DAYS COMPLETED
  *** COMPUTATION AT  93.32     DAYS COMPLETED
  *** COMPUTATION AT  98.32     DAYS COMPLETED
  *** COMPUTATION AT  103.3     DAYS COMPLETED
  *** COMPUTATION AT  108.3     DAYS COMPLETED
```

{other similar messages omitted}

```
  *** COMPUTATION AT  553.3     DAYS COMPLETED
  *** COMPUTATION AT  603.3     DAYS COMPLETED
  *** COMPUTATION AT  653.3     DAYS COMPLETED
  *** COMPUTATION AT  703.3     DAYS COMPLETED
  *** COMPUTATION AT  753.3     DAYS COMPLETED
  *** COMPUTATION AT  803.3     DAYS COMPLETED
  *** COMPUTATION AT  853.3     DAYS COMPLETED
  ***
  *** OUTPUT FILE:
  ***    BENZENE1.TSG
  *** PLOT FILE:
  ***    BENZENE1.PMP
  *** TSGPLUME END
```

1.10 Plotting HSSM Results with HSSM-PLT

The HSSM-PLT program is a graphics post-processor for the HSSM program. HSSM-PLT provides the model users with on-screen visualizations of the output as well as optional hard copies. All inputs are made through a menu, enabling the user to concentrate on the model's results. HSSM-PLT program is written in Microsoft FORTRAN 77 version 5.0 and uses the INGRAF version 5.02 library of FORTRAN graphics routines.

1.10.1 Package Requirements

The plotting program is made up of the three files shown in Table 81. These are supplied on the HSSM-1-d diskette and should be installed in the HSSM directory according to Appendix Table 41.

Table 81 Required Files for the HSSM-PLT Graphical Display Program

File	Function
HSSM-PLT.EXE	The HSSM Graphical Display program
CONFIG.PLT	User supplied information about the printer hardware of the system
SIMPLEX1.FNT	The Sutrasoft font file for lettering the displays.

All three files must be present in the same subdirectory for HSSM-PLT to work properly.

1.10.2 Overview

HSSM-PLT was written with the INGRAF graphics library. The program displays a copyright notice that will appear for approximately two seconds. The Sutrasoft copyright notice is displayed in compliance with the licensing agreement for the INGRAF graphics library. For more information about INGRAF contact:

Sutrasoft (The Librarian, Inc.)
10506 Permian Dr.
Sugarland, TX 77487
(713) 491-2088
FAX (713) 240-6883

HSSM-PLT displays a menu of choices which includes options to 1) exit the program, 2) configure output devices, 3) select HSSM-KO and HSSM-T results files for plotting, and 4) select graphs for display. Options 2 through 4 display either screen messages or additional menus to guide the user.

Table 82 lists the HSSM-PLT command sequence for graphing the results. The full details of the procedures are described in the following sections.

Table 82 Quick Summary of HSSM-PLT Commands		
Step	Command or Menu Item	Action
0	see Table 41	Generate HSSM results
1*	Item 2	Select printer
2	Item 3	Select HSSM-KO and HSSM-T output files
3	Item 4	Graph results
4	press P	Print the graph which is displayed
5	Item 0	Exit

*The printer selection is saved for future use of the program, so step 1 is executed only when the printer is selected initially or changed; or when writing to disk files.

Title Screen

This screen shows the title, version number, and authorship information for the program. This data stays on the screen until the user presses any key.

Menu Screen

The Menu Screen contains the user interface for all the HSSM-PLT program options. To make a selection, the user presses the indicated key for the desired selection. For example, to exit the program a "0" (zero) key is pressed and the program ends. The legal selections are 0 through 3 and any other key strokes are ignored.

Menu Option 1: Device Configuration

The Device Configuration option allows users to select the appropriate output device for his/her system. The configuration data is stored in the **config.plt** file, so the user need only use this option when running the program for the first time, when changing the printer, or when plotting to a disk file. The current output device is displayed on the first line of Table 83. All of the supported output devices are displayed with an index number. By entering the index number, the user selects an output device from the displayed list.

Table 83 Output Device Configuration Options

```
 THE CURRENT OUTPUT DEVICE IS Postscript printer


SELECT AN OUTPUT DEVICE

                1 - EPSON 9-pin, narrow carriage
                2 - EPSON 24-pin, LQ series, narrow
                3 - EPSON 24-pin, LQ series, wide
                4 - NEC Pinwriter, 24-pin, narrow
                5 - NEC Pinwriter, 24-pin, wide
                6 - Okidata, 9-pin, narrow
                7 - HP LaserJet/DeskJet - low res
                8 - HP LaserJet/DeskJet - medium res
                9 - HP LaserJet/DeskJet - high res
               10 - HP PaintJet - 2 color, low res
               11 - HP PaintJet - 4 color, med res
               12 - HP PaintJet - 8 color, high res
               13 - HP PaintJet - 16 color, high res
               14 - Postscript printer
               15 - HP - HPGL plotter
               16 - HP LaserJet III - HPGL/2 mode
               17 - Houston Inst DM/PL plotter

 ENTER DEVICE NUMBER :
```

After the output device selection is made, the output port is assigned (Table 84). The screen follows the same format as for the device: The current port is shown, followed by the possible port selections. By entering the index number, the user selects an output port from the displayed list.

Table 84 Output Device Port Selection

```
THE CURRENT OUTPUT PORT IS LPT1:


 SELECT AN OUTPUT PORT


               1 - PRN:
               2 - LPT1:
               3 - LPT2:
               4 - COM1:
               5 - COM2:
               6 - AUX:
               7 - FILE


 ENTER PORT NUMBER:
```

Option 7 sends the graph to an HPGL format disk file rather than an output device. When this option is selected, the user is prompted for a filename in addition to the port number. Note that only the last graph written to file is retained in the file. If more than one graph is desired to be written to a file, the configuration must be reentered each time for each graph in order to change the name of the output file.

Menu Option 2: Selecting Input Files

Before graphing results, a set of HSSM results must be selected. All of the necessary plot files are read by HSSM-PLT and become available for drawing specific graphs. If graphing is attempted before selecting the plot files, a reminder to select a file is given.

The first message that appears on the screen is

```
ENTER SUBDIRECTORY PATH NAME
PRESS <ENTER> TO USE CURRENT DIRECTORY:
```

The user may then press <ENTER> to use the current directory, or supply a DOS path name such as c:\models\hssm\working

The user is prompted for a file name by the following message:

```
ENTER FILE NAME OR  * FOR A DIRECTORY
USE THE ROOT ONLY - NO EXTENSIONS:
```

Pressing <ENTER> or an asterisk displays the current directory of HSSM-KO input files (files with extension **.DAT**). Entering the root name, such as BENZENE, causes HSSM-PLT to begin reading the plot files. HSSM-PLT adds the extensions to the root file name when it retrieves the plot files. For this example, the following messages were written to the screen:

```
READING FILE  c:\models\hssm\working\BENZENE.PL1 ....  DONE
READING FILE  c:\models\hssm\working\BENZENE.PL2 ....  DONE
READING FILE  c:\models\hssm\working\BENZENE.PL3 ....  DONE
FILE c:\models\hssm\working\BENZENE.PMP  DOES NOT EXIST
READING FILE  c:\models\hssm\working\BENZENE.HSS ....  DONE


PRESS ANY KEY TO CONTINUE
```

The plot files **BENZENE.PL1, BENZENE.PL2, BENZENE.PL3** and the main result file **BENZENE.HSS** were read successfully. The HSSM-T plot file **BENZENE.PMP** did not exist as HSSM-T had not been run for this data set.

Menu Option 3: Selecting Graphs

After the input file has been selected, graphs can be generated. Option 3 from the main menu brings up the graph menu. If no input file has been selected then an error message is displayed. The legal entries for the graph menu are 0 - 7 and all other key strokes will be ignored. Each of the graphs is described in detail in the next section. Generally, after the graph is drawn on the screen, pressing any key will bring the user back to the graphics menu. However, if the user presses the <P> key, the graph will be printed according to the data in the **CONFIG.PLT** file.

1.11 Graphical Presentation of HSSM Output

Two basic types of graphs are produced by the DOS graphics post-processor. These are profiles which present the spatial variation of a parameter at a given time, and histories which present the time variation of a parameter at a given location. The graphics present a visual summary of the output from a successful HSSM simulation. Results from each of the modules of HSSM are contained in one or more of the graphs. **(35)** gives information on each of the graphs provided.

Table 85 HSSM Graphics

Graph Number	Title	HSSM Module	Description
1	Saturation Profiles	KOPT	Vadose zone liquid saturations from the surface to the water table
2	NAPL Front Position History *	KOPT	Location of the NAPL front in the vadose zone
3	NAPL Lens Profiles	OILENS	Cross-section of the NAPL lens on the water table
4	NAPL Lens Radius History	OILENS	History of the radius of the NAPL lens and the effective radius of the contaminant
5	Contaminant Mass Flux History	OILENS	History of the mass flux from the NAPL lens to the aquifer
6	NAPL Lens Contaminant Mass Balance	OILENS	History of the mass in the NAPL lens
7	Receptor Concentration Histories	TSGPLUME	History of the contaminant concentrations at the receptor points

* Only the MS-DOS interface produces the NAPL Front Position History.

The graphs produced by HSSM-PLT are very similar to those produced by HSSM-WIN. Examples of the HSSM-WIN graphs are shown in Section 4.8.

Appendix 2 DOS Example Problem

In this Appendix, an example problem is presented that illustrates the use of the DOS interface. This problem is the same as the first example presented in Section 5. The complete set of input and output files for this example is distributed on the HSSM-2 diskette.

2.1 Gasoline Arrival Time at the Water Table

An emergency response and monitoring plan is being prepared for an above ground storage tank facility. An estimate is needed of how long it would take gasoline to reach the water table and what monitoring frequency would be required to detect a leak before gasoline reaches the water table. The soil has been classified as a sandy clay loam soil. In this example, the water table lies at a depth of 5.0 meters. All of the parameters for the model run are saved in the file **X1STF.DAT**, which is found on the example problems diskette HSSM-2. PRE-HSSM can be used to page through this file as the example is studied.

This problem needs the use of the KOPT module with no dissolved contaminant. A "per unit area" simulation should be performed because only the transport time through the vadose zone is required. The MS-DOS interface will be used to demonstrate how HSSM is used for this problem. Of all the input data required for the model, only the following parameters are required for the "KOPT only" simulation. PRE-HSSM places necessary zeros in the data file for the unused parameters.

Screen 1. Printing Option Switches

Only the output file production and KOPT options are used in the example simulation as shown in Table 86.

Table 86 Problem 1 Printing Option Switches

Parameter	Rationale	Value
IWR	Produce Output files	1
IKOPT	Run KOPT	1
ICONC	No dissolved constituent	0
ILENS	Do not run OILENS	0
ITSGP	Do not write HSSM-T input file	0

Screen 2 File Names

The required file names are generated automatically when the data set is saved by PRE-HSSM. The stem for this data set is X1STF.

Screen 3 Run Title

Gasoline Release from an Aboveground Storage Tank Fac.
Gasoline Arrival Time at the Water Table
KOPT Simulation Only

Screen 4 Porous Medium Properties

The porous medium properties listed on Screen 4 are estimated from Brakensiek et al.'s soil parameter tabulation. The values shown in Table 87 are taken from the tabulation reproduced in Appendix 3.1.

Table 87 Problem 1 Porous Medium Properties

Parameter	Value
Air Entry Head, h_{ce}	46.3 cm
Brooks and Corey's Pore Size Distribution Index, λ	0.368
Residual Water Content, θ_{wr}	0.075
Porosity, η	0.406

The hydraulic conductivity in cm/s of the system is then estimated from (Brakensiek et al., 1981)

$$K_s \quad = \quad 270\,\frac{\eta^2}{h_{ce}^2}\,\frac{\lambda^2}{(\lambda + 1)\,(\lambda + 2)} \quad = \quad 8.68\,x\,10^{-4}\ cm/s \tag{36}$$

where the air entry head is in cm. The value is then converted to the units of meters per day by multiplying by 864 to give a K_s of 0.75 m/d. From the basic soil property information, the following parameters are determined (Table 88).

Table 88 Problem 1 Hydraulic Conductivity and Capillary Pressure Curve Parameters

Parameter	Rationale	Value
Ratio of Horizontal to Vertical Conductivity	Arbitrary value as this parameter is not used in KOPT	5.0
Relative Permeability Index	The Brooks and Corey Model is used	1
Air Entry Head, h_{ce}	The required units for HSSM are meters. This parameter is entered on screen 7	0.463 m
Residual Water Saturation, S_{wr}	HSSM requires saturation input rather than "content" input	0.18 (0.075 / 0.406)

Screen 5 Hydrologic Properties

The parameters shown in Table 89 are used for the Hydrologic Properties screen.

Table 89 Problem 1 Hydrologic Properties

Parameter	Rationale	Value
Water Phase Density, ρ_w	Standard value	1.0 g/cm^3
Water Phase Viscosity, μ_w	Standard value	1.0 cp
Recharge Input Type	Specify Saturation	2
Water Saturation, $S_{w(max)}$	Specified water saturation	0.35
Maximum Relative Permeability During Infiltration, $k_{rw(max)}$	Assume 0.5	0.5
Depth of Water Table	Arbitrary for this problem	5 m

The depth to the water table is stated to be arbitrary because KOPT only treats the vadose zone above the water table (and capillary fringe). The model results should be checked for the time at which the NAPL front crosses the 5 meter depth.

Screen 6 Hydrocarbon (NAPL) Phase Properties

Table 90 Problem 1 Hydrocarbon (NAPL) Phase Properties

Parameter	Rationale	Value
Oil Phase Viscosity, μ_o	Typical value for gasoline	0.45 cp
Oil Phase Density, ρ_o	Typical value for gasoline	0.74 g/cm^3
Residual Oil Saturation (vadose zone), S_{orv}	Estimated	0.10
Oil Application Type	Select a constant head ponding scenario	3

Screen 7 Capillary Suction Approximation Parameters

The capillary suction approximation parameters are used to add the effect of capillary suction on the infiltrating NAPL. The air entry head of the Brooks and Corey model (0.46 m) is entered on this screen. The surface tension of water is taken as 65 dyne/cm to account for the fact that the published values of surface tension are for very pure water. The NAPL surface tension is taken to be 35.0 dyne/cm.

Screen 8c Hydrocarbon (NAPL) Constant Head Ponding Boundary Condition

Because the constant head release scenario was chosen on Screen 6, the constant head ponding boundary condition screen appears on screen 8. The beginning time, ending time and ponding time are entered on this screen. The release is assumed to begin at time of 0 days and end at a time of 1 day. During this interval the ponding depth is assumed to remain constant at 0.05 m (5 cm).

Screen 11 OILENS Model Parameters, First Screen

OILENS is not used in the present simulation. The radius of the source must be specified, however, and this parameter is grouped with the OILENS parameters. Only a "per unit area" simulation is desired for this example, so the source radius is set to 0.5642 meters so that the resulting source area is 1.00 meters. None of the other parameters on this screen need to be entered.

Screen 13 Simulation Control Parameters

Table 91 Problem 1 Simulation Control Parameters

Parameter	Rationale	Value
Simulation Ending Time	Simulate the release for 25 days, since gasoline is a low viscosity fluid and can reach the water table relatively rapidly in a permeable media.	25 days
Maximum Solution Time Step	Use a relatively small value, because only 25 days are simulated	0.1 day
Minimum Time Between Printed Time Steps	Use a value smaller that the minimum solution time step.	0.05 day
Ending Criterion	Stop the simulation at the specified time	1
Minimum mass factor	Not used for this simulation	0.01

Screen 14 Number of Profiles and Screen 15 Profile Times

Use 5 profiles during the simulation. The times should be small, since the gasoline is expected to reach the water table relatively rapidly. Use times of 0.25, 0.5, 1.0, 2.0 and 5.0 days (6, 12, 24, 48 and 60 hours).

Model Results

The model is executed by entering the command

```
HSSM-KO X1STF.DAT
```

The saturation profiles from the simulation are shown in **Figure 40**. These profiles were drawn with the HSSM-PLT program. The depth of the sharp front increases with time and the first three profiles show uniform NAPL saturations. The last two profiles show varying NAPL saturations, because they occur at 48 and 60 hours which both are past the end of the release (24 hours). **Figure 41** shows the NAPL front position. This graph indicates that over the 25-day duration of the simulation, the NAPL does not go deeper than about 3.6 meters.

Figure 40 Saturation profiles

Figure 41 The front position

With complete confidence in the accuracy of the input data, it could be assumed that the gasoline never reaches the water table. However, most of the model parameters used in this example have been estimated from published tabulations. Rather than accepting the results of one simulation as being authoritative, several simulations should be run in order to get some feel for the effects of parameter variability. If the hydraulic conductivity was in fact 10 times greater than the average value of 0.75 m/d, the gasoline would flow deeper into the subsurface. Because of the constant head ponding condition assumed for this case, the gasoline would also flow faster. The constant head ponding condition does not specify the volume of gasoline which enters the soil; it only indicates that enough gasoline is supplied to maintain the 0.05 m ponding depth for one day. **Figure 42** shows the NAPL front position when the hydraulic conductivity is 7.5 m/d. By 25 days, the gasoline would reach 24 meters deep, if not for the water table 5.0 meters deep. From the **X2STF.HSS** file, the depth of 5 meters was reached within 9.8 hours.

This example has focussed on the role of the hydraulic conductivity in determining the depth of the gasoline. The effect of variation in other parameters can likewise be demonstrated. Some of the other uncertain parameters are the assumed release condition, moisture content, and capillary pressure parameters.

Figure 42 Storage tank facility example with increased conductivity

Appendix 3 Sources of Parameter Data

The data that are used in models are of crucial importance for determining the quality of the results and their applicability to the real world problems they are intended to simulate. Often where model applications fail to be realistic, the failure is due to data limitations and lack of fundamental understanding of site specific transport processes, both hydrologic and chemical. The following section does not address directly all of these issues, rather it describes the uses and limitations of estimated parameter values. The discussion below is intended to highlight the importance of several HSSM input parameters. Further detailed information on parameter values is given in Section 4.6 for HSSM-WIN and in Appendix 1 for HSSM-DOS. For convenience, both of these sections contain the same information.

Unarguably, the best sources for parameter values are site- and pollutant-specific data obtained under an appropriate quality assurance/quality control program. There is no substitute for measured data. Unfortunately such data are not always available and recourse must be made to estimated or tabulated parameter values. When this type of data is used for modeling, it must be recognized that very significant uncertainty is being introduced into the simulation results. The model results may be useful, however, for addressing such issues as comparison of the effects of various pollutant or soil properties on transport. For example, given a soil type, perhaps defined by parameters selected from a nationwide tabulation, how does the transport of benzene compare with that of toluene? HSSM model results may provide some understanding of relative transport effects. Because of practical and theoretical limitations in understanding subsurface transport, site specific prediction of future contaminant behavior is questionable with any model.

3.1 Soil Properties

Of primary importance are the soil properties: saturated hydraulic conductivity, K_s, and the water/air capillary pressure curve, $P_c(S)$, (a.k.a. the moisture characteristic curve or the moisture retention curve). Note that the term "saturated hydraulic conductivity" refers to the conductivity to water as defined by Darcy's Law:

$$q_w = -K_s \frac{dh}{dl} \qquad \textbf{(37)}$$

where q_w is the water flux, K_s is the hydraulic conductivity, and -dh/dl is the hydraulic (head) gradient. The capillary pressure curve depends on some of the same features of the porous medium as does K_s. These features include the grain and pore size distribution, and the sand, silt, clay and loam fractions. There may be relationships between K_s and parameters describing the $P_c(S)$ curve (Brutsaert, 1967; Brakensiek et al., 1981; Carsel and Parrish, 1988).

Brooks and Corey (1964) presented the following power-law relationship between capillary pressure and reduced saturation

$$\left(\frac{S_w - S_{wr}}{1 - S_{wr}} \right) = \left(\frac{h_{ce}}{h_c} \right)^{\lambda} \qquad \textbf{(38)}$$

where S_{wr} is the irreducible (residual) water saturation, λ is called the pore size distribution index, and h_{ce} is the air entry head. In practice S_{wr}, λ, and h_{ce} are parameters which are fitted to an experimental data set.

van Genuchten (1980) proposed a similar model

$$\frac{\theta_w - \theta_{wr}}{\theta_m - \theta_{wr}} = \left(\frac{1}{1 + (\alpha h)^n} \right)^m \qquad \textbf{(39)}$$

where θ_{wr} is the residual water content, θ_m is the maximum water content, and α, n, and m are parameters. Note that the water content, θ_w, the saturation, S_w, and the porosity, η, are related by

$$\theta_w = \eta \, S_w \qquad \textbf{(40)}$$

θ_{wr}, θ_m, α, n, and m can be parameters which are fitted to an experimental data set. Usually m is taken to be a simple function of n (i.e., m = 1-1/n).

Brakensiek et al. (1981) tabulated Brooks and Corey parameters from a number of soil samples and organized the results by soil classification. The hydraulic conductivity in cm/s was calculated from the following formula from Brutsaert (1967)

$$K_s = C \left(\frac{\theta_m - \theta_{wr}}{h_{ce}} \right)^2 \frac{\lambda^2}{(\lambda + 1)(\lambda + 2)} \qquad \textbf{(41)}$$

where C is a constant taken as 270 by Brakensiek et al. (1981) and as 21 by Rawls et al. (1983). Thus this tabulation consists of measured $P_c(S)$ data fitted to the Brooks and Corey model and calculated K_s values. Table 92 shows Brakensiek et al. (1981) results with their statistical distributions of parameter values. For each parameter, Brakensiek et al. chose the most suitable distribution and presented their result in terms of means and standard deviations of transformed distributions (e.g., log normal). Table 92 shows the untransformed values which would be used directly to generate a capillary pressure curve. These values were developed by using the statistical distributions given by Brakensiek et al. (1981) to generate a distribution of each parameter. The mean values of the distributions were determined and are shown in Table 92. All of the values of the pore size distribution index, λ, are low, which indicates wide pore size distributions (well sorted materials). Some sands, in particular, may be more uniform and be better represented by a higher value. Brooks and Corey parameters for several sands whose capillary pressure curves were measured at RSKERL are presented in Table 93. These examples have higher λ values than does the tabulation.

Table 92 Average Soil Properties Determined from Brakensiek et al. (1981)

Soil Texture Class (number of samples)	λ	h_{ce} (cm)	η	θ_{wr}
Sand (19)	0.573	35.3	0.349	0.017
Loamy Sand (69)	0.460	15.9	0.410	0.024
Sandy Loam (166)	0.398	29.2	0.423	0.048
Loam (83)	0.258	50.9	0.452	0.034
Silt Loam (199)	0.216	69.6	0.484	0.018
Sand Clay Loam (129)	0.368	46.3	0.406	0.075
Clay Loam (112)	0.283	42.3	0.476	0.087
Silty Clay Loam (175)	0.178	57.8	0.473	0.054
Silty Clay (26)	0.212	41.7	0.476	0.085
Clay (108)	0.214	64.0	0.475	0.106

Table 93 Brooks and Corey Parameters for Selected Sands

Sand	h_{ce} (cm)	λ (*)	S_{wr} (*)
Lincoln	42.8	1.69	0.09
Oil Creek	53.9	4.19	0.04
Traverse City	24.0	2.43	0.0
c109	23.7	3.86	0.01
c190	10.2	4.65	0.08

In the Brakensiek et al. tabulation, sand has a higher air entry value (35.3 cm) than loamy sand (15.9 cm). This suggests that Brakensiek et al.'s sand data are dominated by relatively fine sands of wide pore size distribution. Notice also that the clay type has a lower air entry value (64.0 cm) than does the silt loam (69.6 cm). In some of the texture classes only a small number of samples were used to generate the parameter values, which is a probable reason for the anomalous parameters. As a result, the aforementioned features of the tabulation suggest that it may only be useful as a rough guide for estimating parameter values.

Carsel and Parrish (1988) presented a tabulation of data based on van Genuchten's (1980) model and soil texture data. K_s, α, n, θ_{wr}, and θ_m were estimated from regression equations developed previously by Rawls and Brakensiek (1985) for Brooks and Corey parameters. Carsel and Parrish used an asymptotic approximation to convert the Brooks and Corey h_{ce} and λ values to van Genuchten α and n values. The results of the Carsel and Parrish (1988) tabulation are reproduced in Table 94 for the saturated and residual water contents, Table 95 for the parameters n and α, and Table 96 for hydraulic conductivity.

Table 94 Descriptive Statistics from Carsel and Parrish (1988) Data Set

Soil type	Saturated Water Content θ_m			Residual Water Content θ_r		
	sample size	mean	standard deviation	sample size	mean	standard deviation
Clay*	400	0.38	0.09	353	0.068	0.034
Clay Loam	364	0.41	0.09	363	0.095	0.010
Loam	735	0.43	0.10	735	0.078	0.013
Loamy Sand	315	0.41	0.09	315	0.057	0.015
Silt	82	0.46	0.11	82	0.034	0.010
Silt Loam	1093	0.45	0.08	1093	0.067	0.015
Silty Clay	374	0.36	0.07	371	0.070	0.023
Silty Clay Loam	641	0.43	0.07	641	0.089	0.009
Sand	246	0.43	0.06	246	0.045	0.010
Sandy Clay	46	0.38	0.05	46	0.100	0.013
Sandy Clay Loam	214	0.39	0.07	214	0.100	0.006
Sandy Loam	1183	0.41	0.09	1183	0.065	0.017

Table 95 Descriptive Statistics from Carsel and Parrish (1988) Data Set

Soil type	n			α, (m^{-1})		
	sample size	mean	standard deviation	sample size	mean	standard deviation
Clay*	400	1.09	0.09	400	0.80	1.2
Clay Loam	364	1.31	0.09	363	1.9	1.5
Loam	735	1.56	0.11	735	3.6	2.1
Loamy Sand	315	2.28	0.27	315	12.4	4.3
Silt	82	1.37	0.05	82	1.6	0.70
Silt Loam	1093	1.41	0.12	1093	2.0	1.2
Silty Clay	374	1.09	0.06	126	.50	0.50
Silty Clay Loam	641	1.23	0.06	641	1.0	0.60
Sand	246	2.68	0.29	246	14.5	2.9
Sandy Clay	46	1.23	0.10	46	2.7	1.7
Sandy Clay Loam	214	1.48	0.13	214	5.9	3.8
Sandy Loam	1183	1.89	0.17	1183	7.5	3.7

Table 96 Descriptive Statistics from Carsel and Parrish (1988) Data Set

Soil type	Hydraulic Conductivity K_s, (m/d)		
	sample size	mean	standard deviation
Clay*	114	0.048	0.10
Clay Loam	345	0.062	0.17
Loam	735	0.25	0.44
Loamy Sand	315	3.5	2.7
Silt	88	0.060	0.079
Silt Loam	1093	0.11	0.30
Silty Clay	126	0.0048	0.026
Silty Clay Loam	592	0.017	0.046
Sand	246	7.1	3.7
Sandy Clay	46	0.029	0.067
Sandy Clay Loam	214	0.31	0.66
Sandy Loam	1183	1.1	1.4

* The clay type represents an agricultural soil with clay content of 60% or less.

As a third approach to estimating the soil hydraulic properties, Rawls and Brakensiek (1985) developed regression equations for the Brooks and Corey parameters. The required data for use of the regressions are the percent sand, PS, the percent clay, PC, and the porosity, η. The general form of the regression equations is

$$f(PS, PC, \eta) = [b_o + \sum b_{ijk} PS^i PC^j \eta^k] \qquad \textbf{(42)}$$

To apply the regression equations, the percent sand must be between 5 and 70 and the percent clay must be between 5 and 60. Table 97 gives the values of the regression coefficients for estimating the residual water content, θ_r, the natural log of the hydraulic conductivity, K_s, entry head, h_{ce}, and pore size distribution index, λ. Appendix 5 describes a utility program called SOPROP which uses the regression equations to estimate these hydraulic properties.

Table 97 Regression Coefficients from Rawls and Brakensiek (1985)

Coefficient	$\ln(K_s)$	θ_r	$\ln(h_{ce})$	$\ln(\lambda)$
b_o	-8.96847	-0.0182482	5.3396738	-0.784281
b_{100}	--	0.00087269	--	0.0177544
b_{010}	-0.028212	0.00513488	0.1845038	--
b_{001}	19.52348	0.02939286	-2.48394546	-1.062498
b_{200}	0.00018107	--	--	-0.00005304
b_{020}	-0.0094125	-0.00015395	-0.00213853	-0.00273493
b_{002}	-8.395215	--	--	1.11134946
b_{110}	--	--	--	--
b_{101}	0.077718	-0.0010827	-0.0435649	-0.03088295
b_{011}	--	--	-0.61745089	--
b_{210}	0.0000173	--	-0.00001282	-0.00000235
b_{021}	0.02733	0.00030703	0.00895359	0.00798746
b_{201}	0.001434	--	-0.00072472	--
b_{120}	-0.0000035	--	0.0000054	--
b_{012}	--	-0.0023584	0.50028060	-0.00674491
b_{202}	-0.00298	--	0.00143598	0.00026587
b_{022}	-0.019492	-0.00018233	-0.00855375	-0.00610522

Before continuing, the accuracy of using tabulated "average" parameter values is illustrated through a comparison of measured capillary pressure curves with the average for sand. **Figure 43** shows the average curve for Brakensiek et al.'s sand and data from several sands measured at RSKERL using a technique developed by Su and Brooks (1980). These sands are not meant to be a representative sample, but were materials used in several experiments. The class "sand" is seen to contain much variability and the average curve does not necessarily represent any particular sand.

The 20/30, C109 and "Texas" sands are commercial products with relatively uniform pore size distributions. The curves appear almost as step functions. The TCS sand from Traverse City, Michigan, and the Lincoln and Oil Creek sands, both from Pontotoc County, Oklahoma, are natural materials. Oil Creek has a uniform pore size distribution and is not very representative of sands in general. The Lincoln has a wider distribution of pore sizes than the others and has a less abrupt curve. The Carsel and Parrish average curve has a much lower air entry head, suggesting that their data set was dominated by coarse sands. Data, such as shown in **Figure 43**, may be fitted to either of the capillary pressure models by non-linear curve fitting procedures. The model called <u>Ret</u>ention <u>C</u>urve (RETC) by van Genuchten et al. (1991) is a special purpose program for fitting these models to data.

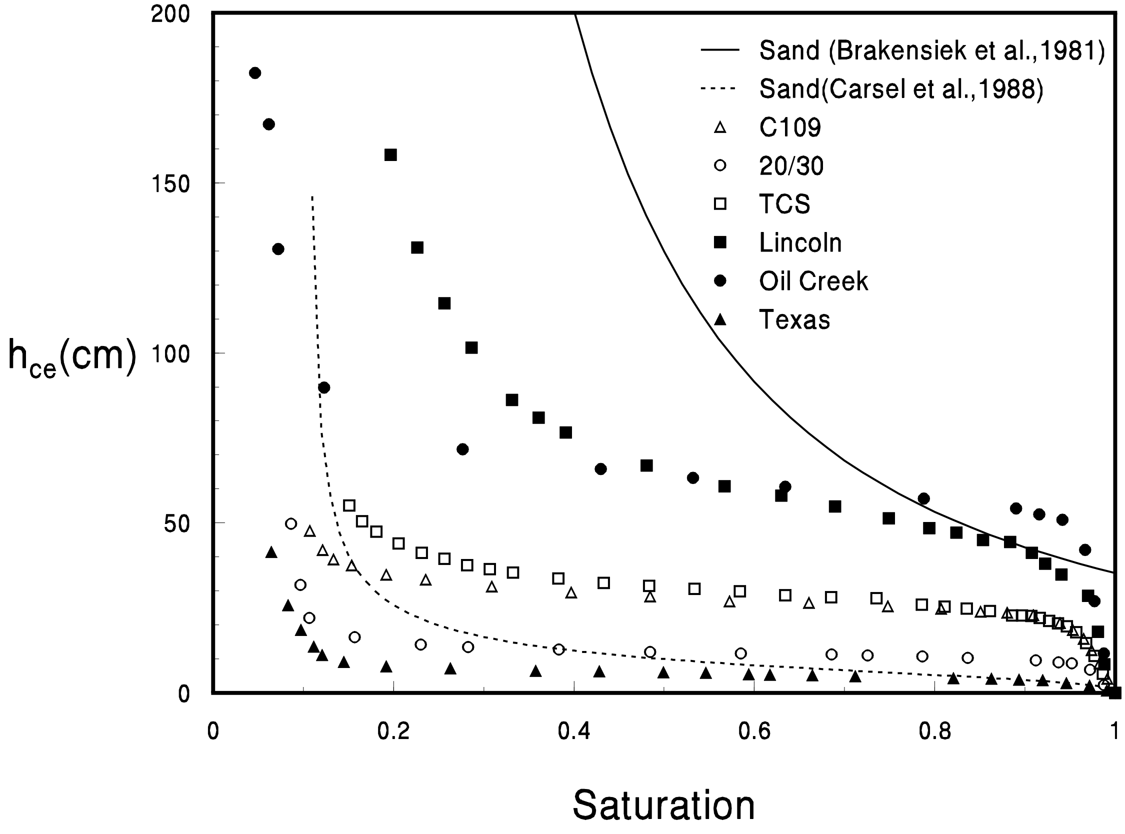


Figure 43 Comparison of average capillary pressure curves with measured data

3.2 NAPL/Water Partition Coefficient

Partitioning of chemicals constituents which compose the NAPL between the NAPL and water phase is another phenomena of major importance. In HSSM this partitioning is assumed to follow a linear equilibrium relationship

$$c_o = K_o \, c_w \tag{43}$$

where c_o is the concentration in NAPL, c_w is the concentration in water, and K_o is the dimensionless NAPL/water partition coefficient. The magnitude of this coefficient has a major influence on the model results as it partially determines how much of the chemical is released from the NAPL to the water.

K_o depends on the composition of the NAPL. Based on their work with 31 gasoline samples, Cline et al. (1991) suggest that Raoult's Law can be used to estimate K_o for gasoline mixtures. Raoult's Law provides an estimate of K_o for the k^{th} constituent of a NAPL that is composed of a total of j constituents as

$$K_o = \frac{\omega_k \sum \frac{c_{oj}}{\omega_j}}{s_k \; \gamma_k} \tag{44}$$

where ω_j is the molecular weight of the j^{th} constituent (g/mol), c_{oj} is the concentration of the j^{th} constituent in the oil phase (g/L), s_k is the solubility of species k in water (g/L), and γ_k is the activity coefficient of the k^{th} species. The activity coefficients equal 1.0 for ideal solutions. Equation **(44)** indicates that the magnitude of K_o depends on the composition of the NAPL, so it is not possible to tabulate values of K_o for universal application. Table 98 contains partitioning and solubility data for several organic compounds of interest.

Table 98 Partitioning Characteristics ([a]Mercer et al., 1990, [b]Cline et al., 1991, [c]Chemical Information Systems, 1994)

Constituent	Water Solubility (mg/L)	K_{oc} (mL/g) or (L/kg)
benzene[a]	1750	83
ethylbenzene[a]	152	1100
toluene[a]	535	300
m-xylene[a]	130	982
o-xylene[a]	175	830
p-xylene[a]	196	870
MTBE methyl *tert*-butyl ether	48000[b]	11.2[c]

The compositional dependence of K_o presents a problem in that K_o varies with the composition of the NAPL: gasoline, diesel, fuel, oil, etc. In order to apply equation **(44)** the concentration C_{oj} of each component or general class of components in the NAPL mixture must be known. Further, as more soluble components of the NAPL are lost, K_o may change. Cline et al.'s (1991) measured partition coefficients for benzene and toluene, however, showed only a slight variation with concentration.

Baehr and Corapcioglu (1987) used a simplified mixture to represent gasoline which is shown in Table 99. From this composition several K_o's are calculated from equation **(44)** and are listed in Table 100. Note that benzene, toluene and *o*-xylene are all hydrophobic, but the degree of hydrophobicity varies widely. Included in the tables are data for methyl *tert*-butyl ether (MTBE), an octane enhancer which may occupy up to 15% of gasoline by volume (Cline et al., 1991). The values calculated by using the mixture of Baehr and Corapcioglu (1987) compare favorably with the values measured by Cline et al.(1991).

Table 99 Pseudo-Gasoline Mixture (Baehr and Corapcioglu, 1987)

Constituent	Initial C_{oj} (g/cm^3)	Molecular weight ω_j
benzene	0.0082 (1.14%)	78
toluene	0.0426 (6.07%)	92
xylene	0.0718 (10.00%)	106
1-hexene	0.0159 (2.22%)	84
cyclohexane	0.0021 (0.29%)	84
h-hexane	0.0204 (2.84%)	86
other aromatics	0.0740 (10.31%)	106
other paraffins (C_4-C_8)	0.3367 (46.91%)	97.2
heavy ends (> C_8)	0.1451 (20.21%)	128

Table 100 Fuel/Water Partition Coefficients Measured by Cline et al. (1991) compared with K_o values calculated from Corapacioglu and Baehr (1987) in parentheses.

Constituent	Average K_o	Coefficient of variation % dev.
MTBE methyl *tert*-butyl ether	15.5	19
benzene	350 (312)	21
toluene	1250 (1202)	14
ethylbenzene	4500	13
m-,p-xylene	4350	12
o-xylene	3630 (4440)	12
n-propylbenzene	18500	30
3-,4-ethyltoluene	12500	19
1,2,3-trimethylbenzene	13800	20

Assuming ideality, Cline et al. (1991) used a further approximation to Raoult's law, which can be stated as

$$K_o = \frac{1 \times 10^6 \left(\dfrac{\rho_o}{\omega^o} \right)}{\dfrac{s_k}{\omega_k}} \qquad \textbf{(45)}$$

where ρ_o is the NAPL phase density (g/ml), ω^o is the average molecular weight of the NAPL phase (g/mol), ω_k is the molecular weight of constituent k (g/mol), and S_k is the solubility of the constituent of interest in mg/L. Cline et al.(1991) demonstrated that this approximation provided an adequate fit to the measured partition coefficients from their 31 samples of gasoline. Cline et al. used an average gasoline density of 0.74 g/ml and average gasoline molecular weight of 100-105 g/mol. The measured partition coefficients showed approximately 30% variation, and the fitted Raoult's law relationship adequately represented the trend of the values on a log-log plot. Appendix 6 describes a utility program called RAOULT which performs the Raoult's law calculations using equations **(44)** and **(45)**.

In addition to the partition coefficient, the composition of the NAPL is important in determining the constituent concentrations in the contaminated ground water. Since the water phase concentration depends on the oil phase concentration, the composition of the NAPL dictates both the partition coefficient and the amount of constituent that is available for contamination of the water phase.

3.3 Estimation of the Maximum NAPL Saturation in the Lens

When LNAPL accumulates in a lens it displaces water from the capillary fringe and from below the water table. Not all of the wetting phase is displaced, and the LNAPL saturation increases from the base of the lens towards the top. The distribution of LNAPL near the water table is determined by the forces of gravity and capillarity, and by the dynamics of water table fluctuations. The usual way of monitoring LNAPL thickness is through observation wells. Under conditions where the water table is static, these observation wells record the true energy distribution within the formation, independent of capillary forces. Because the observation wells have a large radius, the capillary pressure is negligible. When the water table fluctuates, such as in a tidal environment, the observation well LNAPL thickness may show little resemblance to the actual thickness within the formation (Kemblowski and Chiang, 1990). HSSM assumes that the water table is static and requires that an average LNAPL saturation within the lens be estimated. This appendix outlines the method for estimating the average LNAPL saturation and Appendix 7 describes the NTHICK utility for performing these calculations.

The maximum LNAPL phase saturation in the lens is determined through approximation of the LNAPL distribution in the capillary fringe. The soil moisture retention curve gives the distribution of water in a two-phase, air-water system, which using the Brooks and Corey model is

$$\Theta_w = \left(\frac{S_w - S_{wr}}{1 - S_{wr}} \right) = \left(\frac{h_{ce}}{z} \right)^{\lambda} , \quad z > h_{ce} \tag{46}$$

where z is measured upward from the water table and Θ_w is the reduced water saturation. At elevations below the entry head, h_{ce}, Θ_w is equal to one. Equation **(46)** gives the reduced water saturation as a function of elevation above the water table under conditions of vertical equilibrium. To apply this model to a multiphase system that includes free product at the water table, one must determine how the equilibrium behavior for an air-LNAPL and LNAPL-water system can be estimated from those for the air-water system. If changes in the soil structure (swelling, etc.) are neglected, then the difference in behavior from one fluid system to another can be attributed only to differences in fluid properties. The development of expressions for relationships between the fluid distributions begins with the Brooks and Corey parameters for the air-water system: h_{ce}, λ and S_{wr}. For multiple fluid systems the subscripts 'w', 'o' and 'a' designate the water, NAPL and air phases. The first generalization of equation **(46)** gives relationships for the entry pressures in a system composed of fluids i and j

$$p_{bij} = p_{baw} \frac{\sigma_{ij}}{\sigma_{aw}} = \rho_w g \, h_{ce} \frac{\sigma_{ij}}{\sigma_{aw}} \tag{47}$$

where p_{bij} is the bubbling (or entry) pressure in a system composed of fluids i and j, σ_{ij} is the interfacial tension between fluids i and j, and g is the acceleration of gravity. p_{baw} is the entry pressure that is associated with the entry head, h_{ce}. Equation **(47)** follows from the assumption that the maximum pore size remains constant and that the entry pressure depends only on the surface tension. The capillary pressure between fluids i and j, p_{cij} is defined by

$$p_{cij} = \Delta\rho_{ij} \, g \, z \tag{48}$$

where $\Delta\rho_{ij}$ is the difference in density between fluids i and j, and the datum z is chosen at the elevation where the capillary pressure vanishes. This gives

$$\Theta_j = \left(\frac{\rho_w h_{ce} \sigma_{ij}}{\Delta\rho_{ij} \sigma_{aw} z} \right)^{\lambda} = \left(\frac{h_{ceij}}{z} \right)^{\lambda} \qquad \textbf{(49)}$$

for $z \geq h_{cij}$ where j is the wetting phase and

$$h_{ceij} = \frac{\rho_w h_{ce} \sigma_{ij}}{\Delta\rho_{ij} \sigma_{aw}} \qquad \textbf{(50)}$$

Similar scaling relationships were introduced by Leverett (1941) and later used by van Dam (1967), Schiegg (1985), Parker et al. (1987), Cary et al. (1989), Demond and Roberts (1991), and others. For the air-NAPL system $\Delta\rho_{ao}$ may be taken as equalling ρ_o, because of the low density of air.

In a three-phase system, water is taken as the wetting fluid, the LNAPL is taken as being of intermediate wettability, while air is the nonwetting fluid. The implication of this wettability order is that water resides in the small pores, LNAPL in the intermediate pores and air in the largest pores. Since the capillary pressure relationships are defined for two-fluid pairs, one has to work with the fluid pairs separately in a three-phase system. This approach has been developed by Leverett (1941) and adopted by Schiegg (1985), Parker et al. (1987) and others. The *Leverett assumption* is that the water saturation in a three phase system depends only on the NAPL-water capillary pressure, while the total liquid saturation, $S_t = S_w + S_o$, is a function of the interfacial curvature of the air-NAPL interface, independent of the number or proportions of liquids contained in the porous medium. With the Brooks and Corey power-law retention model, these relationships may be written as

$$\Theta_w = \Theta_w(p_{cow}) = \left(\frac{h_{ceow}}{z - z_{ow}} \right)^{\lambda} \qquad \textbf{(51)}$$

and

$$\Theta_t = \Theta_t(p_{cao}) = \left(\frac{h_{ceao}}{z - z_{ao}} \right)^{\lambda} \qquad \textbf{(52)}$$

where z_{ow} and z_{ao} are the elevations at which the corresponding capillary pressures would vanish.

Since the LNAPL residual saturations above and below the water table may be different, the scaling functions for the reduced saturations are

$$\Theta_w(p_{cow}) = \frac{S_w - S_{wr}}{1 - S_{wr} - S_{ors}} \tag{53}$$

and

$$\Theta_t(p_{cao}) = \frac{S_t - S_{wr} - S_{orv}}{1 - S_{wr} - S_{orv}} = \frac{S_w + S_o - S_{wr} - S_{orv}}{1 - S_{wr} - S_{orv}} \tag{54}$$

where S_{wr} is the water retention or "field capacity", and S_{ors} and S_{orv} are the residual NAPL saturations in the saturated and vadose zones, respectively.

Together, equations **(51)** through **(54)** determine the fluid distribution near the water table. What is still lacking is a determination of the capillary pressure datums z_{ow} and z_{ao}. However, these are the levels at which one would find the fluid interfaces in observations wells where capillary forces are absent, and the problem reduces to the standard manometer problem from hydrostatics. Let the elevation z_{aw} be that of the free water interface in the absence of NAPL, while z_{ao} and z_{ow} are the corresponding elevations when a NAPL layer of apparent thickness b_o and density ρ_o is present. A simple calculation from hydrostatics shows that

$$z_{aw} - z_{ow} = \frac{\rho_o}{\rho_w} b_o \tag{55}$$

where ρ_w is the density of water. One also finds that

$$z_{ao} - z_{aw} = \left(\frac{\rho_w - \rho_o}{\rho_w} \right) b_o \tag{56}$$

The total thickness of the hydrocarbon present in the free product region, exclusive of any hydrocarbon trapped above or below the water table, is found by integrating the difference between the total liquid content and the water content over the free product region:

$$D_o = \int \left(\theta_t - \theta_w \right) dz \tag{57}$$

This usage of the NAPL layer thickness, D_o, corresponds to that of Schwille (1967) who used it for the ratio between the amount of NAPL spreading laterally on the groundwater surface and the area occupied by it. Other authors have referred to the NAPL layer thickness as that which may be observed visually in a laboratory apparatus.

The total liquid and water contents are estimated using a modified form of the Brooks and Corey capillary pressure function with h_c equal to the elevation above the fluid interface as seen in an observation well. The elevation for the water content is measured from the level of the hydrocarbon-water interface while the elevation for the total liquid content is measured from the level of the air-hydrocarbon interface in the well. The nonwetting phase entry heads for the hydrocarbon-water, and air-hydrocarbon fluid systems, h_{ceow} and h_{ceao} respectively, are estimated from

$$h_{ceow} = \frac{\rho_w \, \sigma_{ow}}{(\rho_w - \rho_o) \, \sigma_{aw}} \qquad \textbf{(58)}$$

and

$$h_{ceao} = \frac{\rho_w \, \sigma_{ao}}{\rho_o \, \sigma_{aw}} h_{ce} \qquad \textbf{(59)}$$

where h_{ce} is the normal air entry head for the air-water system. With equations **(51)** to **(54)** the integral in equation **(57)** can be evaluated. The result may be written as

$$D_o = \alpha + \beta(b_o) \, b_o \qquad \textbf{(60)}$$

where

$$\alpha = \frac{\eta \left[\left[\lambda \left(1 - S_{wr} \right) - S_{ors} \right] h_{ceow} - \left[\lambda \left(1 - S_{wr} - S_{orv} \right) \right] h_{ceao} \right]}{1 - \lambda} \qquad \textbf{(61)}$$

$$\begin{aligned} \beta(b_o) = {} & \eta (1 - S_{wr}) + \frac{\chi}{1 - \chi} \eta \, S_{orv} \\ & - \frac{\eta (1 - S_{wr} - S_{ors})}{1 - \lambda} \left(\frac{(1 - \chi) \, h_{ceow}}{b_o} \right)^{\lambda} \end{aligned} \qquad \textbf{(62)}$$

$$\chi = \frac{\sigma_{ao}}{\sigma_{ow}} \left(\frac{\rho_w - \rho_o}{\rho_o} \right) \left(\frac{1 - S_{wr} - S_{orv}}{1 - S_{wr} - S_{ors}} \right)^{1/\lambda} \qquad \textbf{(63)}$$

Similar results have been presented by Farr et al. (1990) and Parker and Lenhard (1989). In equation **(60)**, b_o is the hydrocarbon layer thickness one would see in a large capillary (observation well), and S_{orv} and S_{ors} are the residual hydrocarbon saturations above and below the lens, respectively. The function $\beta(b_o)$ has only a weak dependence on b_o, especially at moderate to large LNAPL layer thicknesses. This implies that the relationship between D_o and b_o is nearly linear. The ratio of the averaged formation thickness, D_o , and the observation well thickness, b_o, gives the average NAPL saturation in the lens

$$S_{o(\max)} \quad = \quad \frac{D_o}{\eta\, b_o} \quad = \quad \frac{1}{\eta}\left(\frac{\alpha}{b_o} + \beta\right) \qquad \textbf{(64)}$$

Appendix 4 Approximate Conversion of Capillary Pressure Curve Parameters

KOPT and OILENS are designed primarily to use Brooks and Corey's model, however, HSSM-KO allows the entry of van Genuchten capillary pressure parameters. These are not used directly by the model but rather are automatically converted into approximately equivalent Brooks and Corey parameters by a method proposed by Lenhard et al. (1989). Since van Genuchten's model is not equivalent in form to the Brooks and Corey model, the parameters are not exactly equivalent. The conversion is given by

$$\lambda = \frac{m}{1-m} \left(1 - 0.5^{\frac{1}{m}}\right) \tag{65}$$

$$h_{ce} = \frac{S_*^{\left(\frac{1}{\lambda}\right)}}{\alpha} \left(S_*^{\left(\frac{-1}{m}\right)} - 1\right)^{1-m} \tag{66}$$

where

$$m = 1 - \frac{1}{n} \tag{67}$$

and S_* is defined by Lenhard et al.'s (1989) empirical relation

$$S_* = 0.72 - 0.35 \; exp \; (-n^4) \tag{68}$$

Figure 44 and **Figure 45** compare the Brooks and Corey model with van Genuchten's model for equivalent parameter sets. The equivalent parameter sets are shown in Table 101.

Table 101 Equivalent Capillary Pressure Curve Parameters

Soil Texture			Brooks and Corey		van Genuchten	
	θ_m	θ_r	λ	h_{ce}	n	α
Sand	0.43	0.0443	1.1852	4.628	2.7953	0.1417
Sandy Clay loam	0.39	0.1121	0.3887	8.0941	1.4321	0.0858

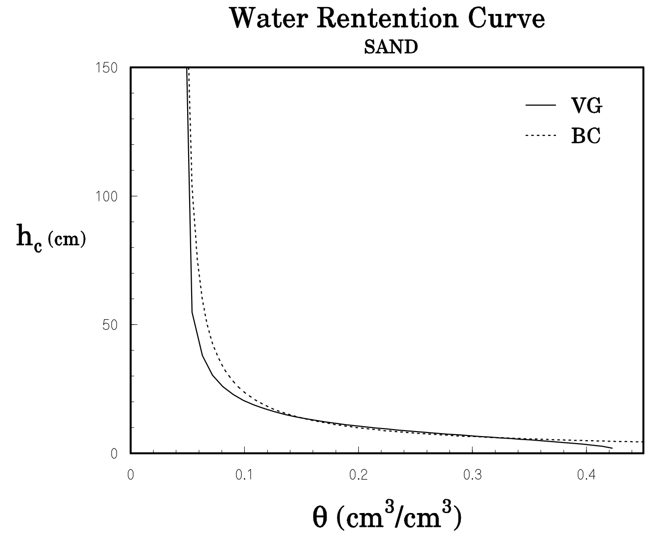


Figure 44 Comparison of equivalent Brooks and Corey and van Genuchten parameters for sandy soil

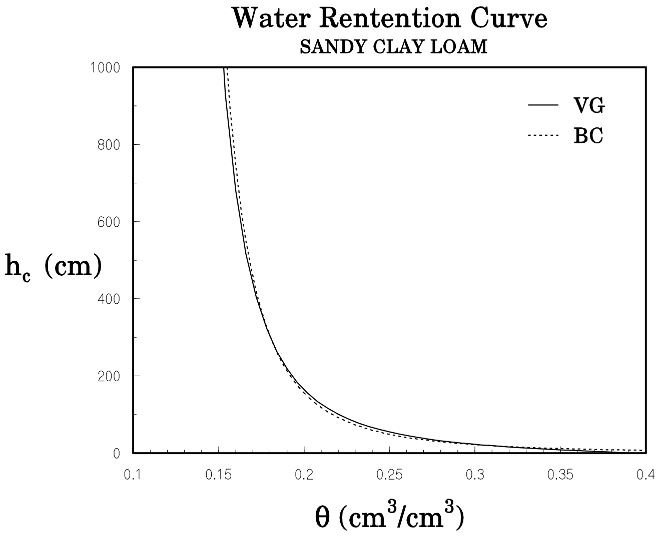


Figure 45 Comparison of equivalent Brooks and Corey and van Genuchten parameters for sandy clay loam soil.

Appendix 5 The Soil Property Regression Utility (SOPROP)

The SOPROP utility is provided with HSSM in order to estimate soil properties from the set of regression equations developed by Rawls and Brakensiek (1985). SOPROP is executed from the DOS prompt by the command:

```
SOPROP
```

No input or output files are required as all the input to and output from the utility are directed to the screen. The user is prompted for 1) the percent sand, PS , 2) the percent clay, PC, and 3) the porosity, η. The hydraulic conductivity and Brooks and Corey parameters are calculated and then written to the screen as shown in Table 102. Recall that the data upon which the regression equations are from agricultural and forest soils; so the SOPROP output is appropriate for similar soils with percent sand between 5.0 and 70.0 and percent clay between 5.0 and 60.0.

Table 102 SOPROP Screen Output

```
*********************************************
Estimate of soil hydraulic properties
from Rawls and Brakensiek (1985)
regression equations
*********************************************
for the soil with:
   70.0000 percent sand
    5.0000 percent clay
     .3500 porosity
the estimated hydraulic parameters are:


hydraulic conductivity            .4257 m/d
Brooks and Corey parameters:
residual water saturation         .1403
air entry head                    .1754 m
pore size distribution index      .4902



     ***successful execution of soprop
```

The range of parameter values that are produced by these equations are shown in Table 103. One extreme occurs when the percent sand is at its maximum value (70%) and the percent clay is at its minimum value (5%). The hydraulic conductivity, as expected, is highest (0.92 m/d) with highest porosity (0.40). Hydraulic conductivities greater than this value are out of the range of the tabulated parameters which form the basis for the regression equations. Likewise another extreme occurs when the percent sand is a minimum (5%) and the percent clay is a maximum (60%). With low porosity (0.30) the conductivity is low (2.3×10^{7} m/d) and the air entry head is high (6.4 m).

Table 103 Range of parameter values produced by the Rawls and Brakensiek (1985) regression equations

SOPROP input parameters			SOPROP results			
Percent sand	Percent clay	Porosity	K_s (m/d)	S_{wr}	h_{ce} (m)	λ
70	5	0.40	0.92	0.12	0.14	0.46
70	5	0.35	0.43	0.14	0.18	0.49
70	5	0.30	0.18	0.18	0.24	0.53
70	5	0.25	0.065	0.22	0.33	0.58
5	60	0.50	1.5×10^{-3}	0.21	1.3	0.12
5	60	0.40	1.3×10^{-5}	0.16	2.9	0.053
5	60	0.30	2.3×10^{-7}	0.023	6.4	0.015

Appendix 6 The RAOULT Utility

Calculation of the NAPL/water partition coefficient, K_o, is simplified through the usage of the RAOULT utility. This utility uses the composition of the hydrocarbon phase for determining the partition coefficient with equations **(44)** and **(45)**. The utility is executed by typing

```
RAOULT
```

at the DOS prompt. The program automatically reads a default data set for gasoline and begins execution of the program.

Table 104 shows the default data set screen messages written by RAOULT. The data is taken from Baehr and Corapcioglu (1987) and is contained in the file **RAOULT.DAT**. The data file may be edited or the data changed interactively by entering a 'Y' at the "Change the input data ?" prompt. The procedures for changing the data are given below.

Table 104   RAOULT Utility Main Screen

```
    **************************************************
    Raoults Law Partitioning Calculation
    **************************************************


    Chemical             Solubility Conc.      Molecular  Activity
                           (mg/L)   (g/cm3)    Weight     Coefficient
    ==================== ========== ========== ========== ==========
  1 benzene               1750.0000      .0082    78.0000     1.0000
  2 toluene                535.0000      .0426    92.0000     1.0000
  3 xylenes                167.0000      .0718   106.0000     1.0000
  4 1-hexene                  .0000      .0159    84.0000     1.0000
  5 cyclohexane               .0000      .0021    84.0000     1.0000
  6 n-hexane                  .0000      .0204    86.0000     1.0000
  7 other_aromatics           .0000      .0740   106.0000     1.0000
  8 other_paraffins           .0000      .3367    97.2000     1.0000
  9 heavy_ends                .0000      .1451   128.0000     1.0000

Change the input data ? (Y or N)
```

With no changes in the input data set (answer 'N' to the "Change the input data ?" prompt, see Table 105), RAOULT determines the density of the hydrocarbon and its average molecular weight. These quantities are used to calculate the hydrocarbon/water partition coefficient using equations **(44)** and **(45)**. The two results are similar and are denoted as determined by the composition basis and the average molecular weight basis, respectively. The user has the option of calculating partition coefficients for other constituents or exiting the utility.

Table 105 Sample RAOULT Calculation for the Benzene Constituent of Gasoline

```
Change the input data ? (Y or N)
N

    Hydrocarbon density    =      .7168
    Avg. Molecular Weight =   104.0458


Select constituent of interest by number
1


    Calculated Hydrocarbon/Water Partition Coefficient:
    Composition basis:
      311.6757
    Average molecular weight basis:
      307.0647


Exit ? (Y or N)
Y

        *** successful execution of raoult
```

The default hydrocarbon composition can be changed by direct editing of the **RAOULT.DAT** data file. The default data set is shown in Table 106. The data set is mostly free format input, with the exceptions noted. The first line contains the number of chemicals composing the hydrocarbon; in this case nine. RAOULT will accept 200 chemicals composing the hydrocarbon phase. The rest of the lines contain the data for each chemical. The chemical name is given first and must be contained within the first 20 spaces of each line. The name may contain any combination of letters, numbers, or other keyboard characters; it may not, however, contain any blanks. In the default data set, blanks are replaced by underscores (as in "other_aromatics"). RAOULT terminates the chemical name at the column where the first number is found, so all 20 of the spaces allocated for the chemical name do not have to be used. Each line contains the following data for the chemical:

- concentration of the chemical in the NAPL in g/cm^3,
- pure compound aqueous solubility of the chemical in mg/L,
- molecular weight of the chemical (g/mol), and
- the activity coefficient.

Here the activity coefficients are taken as being equal to 1.0. Each of the data items must be separated by at least one blank.

Table 106 Default RAOULT.DAT Data Set

```
  9
      benzene          0.0082         1750.    78.    1.
      toluene          0.0426          535.    92.    1.
      xylenes          0.0718          167.   106.    1.
      1-hexene         0.0159            0.    84.    1.
      cyclohexane      0.0021            0.    84.    1.
      n-hexane         0.0204            0.    86.    1.
      other_aromatics  0.0740            0.   106.    1.
      other_paraffins  0.3367            0.   97.2    1.
      heavy_ends       0.1451            0.   128.    1.
```

The data can also be modified interactively within RAOULT by answering 'Y' to the "Change the input data ?" prompt. Table 107 shows the sequence of prompts for changing the benzene solubility from 1750 mg/L to 1780 mg/L and the resulting calculated partition coefficients.

Table 107 Interactive Modification of the RAOULT Default Data Set

```
Change the input data ? (Y or N)
Y

Select item to change by number
1

Select data item to change
1  Name
2  Solubility
3  Concentration
4  Molecular Weight
5  Activity Coefficient
2

Enter the new solubility in mg/L
1780.

Change another data item? (Y or N)
N

    Chemical             Solubility Conc.      Molecular  Activity
                           (mg/L)   (g/cm3)    Weight     Coefficient
    ==================== ========== ========== ========== ==========
  1 benzene              1780.0000      .0082    78.0000     1.0000
  2 toluene               535.0000      .0426    92.0000     1.0000
  3 xylenes               167.0000      .0718   106.0000     1.0000
  4 1-hexene                 .0000      .0159    84.0000     1.0000
  5 cyclohexane              .0000      .0021    84.0000     1.0000
  6 n-hexane                 .0000      .0204    86.0000     1.0000
  7 other_aromatics          .0000      .0740   106.0000     1.0000
  8 other_paraffins          .0000      .3367    97.2000     1.0000
  9 heavy_ends               .0000      .1451   128.0000     1.0000

Change the input data ? (Y or N)
N

    Hydrocarbon density   =      .7168
    Avg. Molecular Weight =   104.0458

Select constituent of interest by number
1

    Calculated Hydrocarbon/Water Partition Coefficient:
    Composition basis:
      306.4227
    Average molecular weight basis:
      301.8895

Exit ? (Y or N)
Y

        *** successful execution of raoult
```

Appendix 7 The NTHICK Utility

A utility program, NTHICK, is provided with HSSM for calculating the averaged LNAPL saturation in the lens, $S_{o(max)}$, based upon the theory presented in Appendix 3.3. NTHICK uses the values from the HSSM-KO input data set to develop a relationship between observation well thicknesses, averaged formation LNAPL thicknesses and the average LNAPL saturations. NTHICK requires a number of parameters taken from the HSSM-KO input data set. These parameters are listed in Table 108 and can be written into the NTHICK input file manually (Table 109). Manual data entry, however, is not necessary because HSSM-KO automatically creates a file with the extension **.NTH** that contains almost all of the NTHICK input parameters. Only the LNAPL/water interfacial tension, σ_{ow}, which is not used by HSSM-KO or HSSM-T, must be added to the **.NTH** file produced by HSSM-KO. NTHICK prompts for the value of σ_{ow} if it is not found in the **.NTH** file, and rewrites the file including the σ_{ow} value as the 5th line of the ***.NTH** file. The program also writes all output to the input data file (***.NTH**). This process does not interfere with later running of NTHICK with the data set; any earlier results are lost, however, when the program is rerun with a previously used input data file.

Table 108 NTHICK required input data

***.NTH** data file line	Parameters
Line 1	Porosity, η
	Air entry head, h_{ce} (m)
	Brooks and Corey's λ
	Residual water saturation, S_{wr}
Line 2	Vadose zone residual LNAPL saturation, S_{orv}
	Aquifer residual LNAPL saturation, S_{ors}
Line 3	Water surface tension, σ_{aw} (dyne/cm)
	LNAPL surface tension, σ_{ao} (dyne/cm)
Line 4	Water density, ρ_w (g/cm^3)
	LNAPL density, ρ_o (g/cm^3)
Line 5	LNAPL/water interfacial tension, σ_{ow} (dyne/cm)

Table 109 NTHICK Input Data File

```
   .4000      0.07    1.500     .10
     .12500     .25
    70.000     30.0000
    1.0000     .7200
   45.0000
```

The result of the program is a list of thicknesses and LNAPL saturations. Table 110 shows a typical set of output messages from NTHICK. The messages are written both to the screen and to the input data file as noted above. First NTHICK echoes the input data set. It follows with the calculated list of observation well thicknesses in meters, averaged formation thicknesses in meters and LNAPL saturations in the lens. The lens thicknesses obviously vary with radius and no one value of $S_{o(max)}$ is exactly correct for the whole lens.

HSSM requires, however, a single value of LNAPL saturation in the lens as input. A procedure for determining a value of $S_{o(max)}$ is given in the following section.

Table 110 Typical NTHICK Output Messages

```
  *********************************************
  Estimate of NAPL saturation in OILENS
  *********************************************

  Porosity                            .4000 (*)
  Air entry head                      .0700 (m)
  Brooks and Corey lambda            1.5000 (*)
  Residual water saturation           .1000 (*)
  Vadose zone residual NAPL sat.      .1250 (*)
  Aquifer residual NAPL sat.          .2500 (*)
  Water surface tension             70.0000 (dyne/cm)
  NAPL surface tension              30.0000 (dyne/cm)
  Water density                      1.0000 (g/cc)
  NAPL density                        .7200 (g/cc)
  NAPL/water interfacial tension    45.0000 (dyne/cm)


  Observation  Averaged        NAPL
      Well     Formation    Saturation
    Thickness  Thickness
     (m)          (m)
  ============ ============ ==========
       .1190      .0005      .0112
       .2690      .0382      .3553
       .4190      .0877      .5230
       .5690      .1404      .6167
       .7190      .1945      .6764
       .8690      .2495      .7177
      1.0190      .3049      .7481
      1.1690      .3607      .7714
      1.3190      .4167      .7898
      1.4690      .4729      .8047
      1.6190      .5292      .8171
      1.7690      .5856      .8276
      1.9190      .6421      .8365

Exit the program ? (Y or N)
```

The "Exit the program ?" prompt at the end of Table 110 either terminates the program by answering "N," or by answering "Y" continues to the estimation of the NAPL saturation for a specific NAPL formation thickness.

Table 111 shows the series of NTHICK prompts that occurs when the program execution continues. The user is asked to enter the NAPL thickness in the formation in meters: here 0.1410 m is used. As shown in Appendix 7.1 below, the NAPL formation thickness is obtained from the HSSM model output. NTHICK responds by echoing the specified average NAPL thickness (.1410) and calculating the associated NAPL lens saturation (.3217).

Table 111 NAPL Saturation Estimation in NTHICK

```
Exit the program ? (Y or N)
n

Enter the average NAPL thickness in the formation (m)
.1410

 Specified avg. NAPL thickness in the formation =      .1410 (m)
 NAPL lens saturation                           =      .3217 (*)
```

7.1 Procedure for Using NTHICK

As noted above, the LNAPL lens saturation depends on the thickness of the lens. A procedure for using NTHICK for determining the lens saturation is given below:

① Develop a data set for HSSM-KO including a trial value of $S_{o(max)}$ and several profile times.

② Run HSSM-KO.

③ Edit the ***.HSS** output file and determine the maximum thickness of the lens. The maximum thickness of the lens can be determined from the lens profiles. The maximum thickness of the lens is read by subtracting the maximum depth of the top and bottom of the lens (columns 4 and 5 of the first row of data in Table 112). The output in this table is from the **X2BT.DAT** data set described in Section 5.2.

If this thickness is not greater than the difference between columns 2 and 3, then the lens has not yet reached its maximum extent and a later profile time must be used. In this case the maximum lens extent from columns 4 and 5 is 10.0943 m - 9.9533 m = 0.1410 m, which is greater than the current lens extent from columns 2 and 3 of 10.0440 m - 9.9729 m = 0.0711 m. Since the maximum lens extent is greater than the current lens extent, this profile can be used for determining the lens thickness and the thickness 0.1410 m is entered into NTHICK.

④ Run NTHICK with the thickness determined from step ③. The thickness is entered interactively in the second part of the NTHICK screen messages (Table 111). NTHICK calculates the associated lens saturation $S_{o(max)}$.

⑤ Average the input $S_{o(max)}$ from step ① and that from step ④.

⑥ Rerun HSSM with the $S_{o(max)}$ determined in step ⑤.

⑦ Repeat until the $S_{o(max)}$ values are within 0.01. If this procedure fails to converge within a few trials, a bisection approach should be used (Forsythe et al., 1977).

Table 112
Lens profile from the *.HSS output file

```
**************************************************
* RADIAL PROFILE THROUGH OIL LENS
**************************************************
TIME                 =   200.0000
LENS RADIUS          =    10.6437
DEPTH TO WATER TABLE =    10.0000

                CURRENT NAPL LENS          MAXIMUM EXTENT OF NAPL LENS
  RADIUS         DEPTH OF        DEPTH OF        DEPTH OF    DEPTH OF
               TOP OF LENS     LENS BOTTOM     TOP OF LENS LENS BOTTOM
==========     ===========     ===========     =========== ===========
    (1)             (2)          (3)           (4)       (5)
     .0000          9.9729         10.0440          9.9533   10.0943
    2.0000          9.9729         10.0440          9.9533     10.0943
    2.4322          9.9739         10.0413          9.9579     10.0827
    2.8644          9.9748         10.0390          9.9617     10.0727
    3.2966          9.9757         10.0368          9.9650     10.0642
    3.7287          9.9764         10.0348          9.9680     10.0567
    4.1609          9.9772         10.0330          9.9704     10.0503
    4.5931          9.9779         10.0312          9.9726     10.0446
    5.0253          9.9785         10.0295          9.9746     10.0397
    5.4575          9.9792         10.0278          9.9762     10.0354
    5.8897          9.9798         10.0262          9.9777     10.0315
    6.3218          9.9804         10.0246          9.9790     10.0282
    6.7540          9.9811         10.0229          9.9802     10.0251
    7.1862          9.9817         10.0213          9.9812     10.0226
    7.6184          9.9823         10.0197          9.9821     10.0202
    8.0506          9.9830         10.0180          9.9830     10.0181
    8.4828          9.9837         10.0162          9.9837     10.0162
    8.9149          9.9844         10.0143          9.9844     10.0143
    9.3471          9.9852         10.0123          9.9852     10.0123
    9.7793          9.9861         10.0099          9.9861     10.0099
   10.2115          9.9873         10.0069          9.9873     10.0069
   10.6437          9.9900         10.0000          9.9900     10.0000

     CUMULATIVE INFLUX TO LENS  1555.


     KOPT AND OILENS GLOBAL MASS BALANCES
     TOTAL NAPL MASS ADDED AT BOUNDARY  (KG)  4091.
     NAPL MASS RECOVERED BY MASS BALANCE (KG) 4059.
     PER CENT ERROR                          -.7962
```

7.2 Example NTHICK Calculation Sequence

Table 113 shows an example sequence of NTHICK and HSSM-KO results which are used to define the input parameter, $S_{o(max)}$. Column (a) lists the trial values of $S_{o(max)}$ that were used in the **X2BT.DAT** data set. In the first trial the value was arbitrarily set to 0.5000. Column (b) gives the maximum NAPL lens thickness in meters as determined from the **X2BT.HSS** file as discussed above. These values were used in NTHICK to determine the appropriate value of $S_{o(max)}$ for the lens (column c). Since the values in columns (a) and (c) do not match (0.5000 vs. 0.2253), the appropriate input value was not used and another trial is needed. The second trial begins with $S_{o(max)}$ set to the average of the previous values in columns (a) and (c), that is 0.5 times (0.5000 + 0.2253) = 0.3627. The sequence of running HSSM-KO, determining the maximum NAPL lens thickness, and estimating the appropriate value of $S_{o(max)}$ continues until the values in column (a) and (c) match fairly closely. In this example it took four iterations to find the correct value of about 0.32 for $S_{o(max)}$.

Table 113 Example sequence of NTHICK and HSSM-KO results

Trial	Initial NAPL Saturation $S_{o(max)}$ (a)	Maximum NAPL lens thickness (b)	NAPL Saturation from NTHICK (c)
1	0.5000	0.0803	0.2253
2	0.3627	0.1219	0.2948
3	0.3288	0.1393	0.3194
4	0.3240	0.1421	0.3231

Appendix 8 The REBUILD Utility

Both of the computational modules of HSSM use temporary files for writing output and plot files. Only at the end of a successful simulation are the temporary files concatenated into output and plot files named as the user has specified. If a simulation is interrupted for any reason, the concatenation of the temporary files will not occur. The user would be left with bits and pieces of the simulation output scattered among the temporary files. The REBUILD utility is designed to create the main output files (**name.HSS** and **name.TSG**) from the temporary files. It also attempts to create the plot files. It is not uncommon, however, that the plot files have incomplete lines or data sets and cannot be plotted. REBUILD does not attempt to recreate the HSSM-T input data file on the assumption that an interrupted simulation cannot have the proper mass flux distribution to run HSSM-T. REBUILD is executed by simply typing

```
REBUILD
```

from DOS or by selecting menu option *(3c)* "Run REBUILD" from Windows. REBUILD uses the temporary files, if they exist, to gather the correct file names for "rebuilding." Thus REBUILD is totally automated.

Appendix 9 Dual Installation of the DOS and Windows Interfaces

Both interfaces can be installed on the same machine by following these instructions:

① Complete the DOS installation process described in Section 1.7.

② Add the HSSM directory to the path as described in Section 1.7.

③ Complete the Windows installation procedure described in Sections 4.3 and 4.3.3. The HSSM directory should be the same as used for the DOS installation.

The dual installation results in one copy each of **HSSM-KO.EXE**, **HSSM-T.EXE** and the other files being copied to the hard drive. All of the components of the interfaces are found in this one directory. HSSM can then be run from any DOS directory or from Windows. DOS and Windows input files can be used with either interface. Windows, however, places the full directory path for the plot and output file names in the HSSM input file (see Table 15). This practice may lead to confusion if the files are later used with the DOS interface, because the output and plot files may be placed in a directory other than that occupied by the input file. The confusion does not arise when using the Windows interface, because HSSM-WIN automatically updates the file names to match the current input file's directory.

Appendix 10 Direct Editing of HSSM-KO Data Files

Sometimes it is convenient to edit data files directly, without using HSSM-WIN or PRE-HSSM. Table 114 shows the items which appear on each line of a valid data file. All data is entered format free; i.e., no special spacing is required, although at least one space must separate each data item. In general an entry is required for each variable given, even for features not used in a particular simulation; therefore, the use of PRE-HSSM or HSSM-WIN for generating input files is recommended.

Table 114 HSSM-KO Input Data File Structure

```
C     ******************************************************************
C     *
C     *  KOPT REQUIRED INPUT DATA
C     *  DATA FILES MAY BE PREPARED OR EDITED BY USING THE PREHSSM
C     *  PREPROCESSOR
C     *
C     *  INPUT ARGUMENTS:
C     *  IRO    READ ONLY INDEX
C     *  IWO    WRITE ONLY INDEX
C     *
C     *  OUTPUT ARGUMENTS: NONE
C     *
C     *  NOTES:
C     *  1.   ALL VARIABLE NAMES ARE IN ACCORDANCE WITH FORTRAN NAM-
C     *       ING CONVENTIONS--NAMES BEGINNING WITH I THROUGH M ARE
C     *       INTEGERS, ALL OTHERS ARE REALS.
C     *  2.   ALL INPUT IS FREE-FORMAT
C     *  3.   ZEROS SHOULD BE READ IN FIELDS PERTAINING TO UNUSED VALUES
C     *  4.   INPUT DATA UNITS ARE SPECIFIED AS FOLLOWS
C     *       (*)       DIMENSIONLESS OR NOT APPLICABLE
C     *       (M)       METERS
C     *       (D)       DAYS
C     *       (C)       DEGREES C
C     *       (CP)      CENTIPOISE  1.0 CP = 0.01 GR/CM/SEC
C     *       (M/D)     METERS PER DAY
C     *       (M2/D)    METERS SQUARED PER DAY
C     *       (MG/L)    MILLIGRAMS PER LITER
C     *       (L/KG)    LITERS PER KILOGRAM SOIL
C     *       (GR/CC)   GRAMS PER CUBIC CENTIMETER
C     *
C     *  LINE 1.....PRINT OUTPUT FLAG....................................
C     *  IWR        OUTPUT WRITING FACTOR                            (*)
C     *             0  SUPPRESS ALL OUTPUT
C     *             1  PRODUCE OUTPUT
C     *  IREO       FOR IWR=1, READ AND ECHO PRINT INPUT DATA ONLY   (*)
C     *             0  READ AND ECHO PRINT INPUT DATA ONLY
C     *             1  RUN MODEL
C     *
C     *  LINE 2-4...RUN TITLE...(5A10/5A10/5A10)........................
C     *  NT(15)     RUN TITLE  3 LINES OF 50 CHARACTERS EACH         (*)
C     *
C     *  LINE 5.....MATRIX PROPERTIES....................................
C     *  WKS        SATURATED VERTICAL HYDRAULIC CONDUCTIVITY (WATER) (M/D)
C     *  RKS        RATIO OF HORIZONTAL TO VERTICAL CONDUCTIVITY    (*)
```

```
C     *  KRF        RELATIVE PERMEABILITY MODEL SELECTION INDEX     (*)
C     *             1 BURDINE--BROOKS & COREY MODEL
C     *  XLAMB      PORE SIZE DISTRIBUTION INDEX                    (*)
C     *             FOR KRF = 1, ENTER LAMBDA
C     *  ETA        POROSITY                                        (*)
C     *  SWR        RESIDUAL WATER SATURATION                       (*)
C     *
C     *  LINE 6.....WATER PROPERTIES....................................
C     *  WMU        DYNAMIC VISCOSITY OF WATER                      (CP)
C     *  WRHO       DENSITY OF WATER                               (GR/CC)
C     *  IRT        RAINFALL INPUT TYPE:  1=FLUX SPECIFIED           (*)
C     *                                   2=SATURATION SPECIFIED     (*)
C     *  QW/SWMAX   CONSTANT WATER FLUX OR SATURATION            (M/D) OR (*)
C     *  XMKRW      MAX WATER RELATIVE PERMEABILITY DURING INFILTRATION (*)
C     *  WTABLE     DEPTH TO WATER TABLE                             (M)
C     *
C     *  LINE 7.....OIL CHARACTERISTICS.................................
C     *  PMU        DYNAMIC VISCOSITY OF OIL                        (CP)
C     *  PRHO       OIL DENSITY                                    (GR/CC)
C     *  SPR        RESIDUAL (TRAPPED) OIL SATURATION                (*)
C     *  IAT        OIL INPUT TYPE  1=FLUX SPECIFIED                 (*)
C     *                             2=VOLUME/AREA SPECIFIED
C     *                             3=CONSTANT PONDING DEPTH
C     *                             4=VARIABLE AFTER CONSTANT PERIOD
C     *
C     *  LINE 8.....CAPILLARY SUCTION APPROXIMATION.(ADDITIONAL PARAMETERS)
C     *  HWE        AIR ENTRY HEAD                                    (M)
C     *  WSIG       WATER SURFACE TENSION                         (DYNE/CM)
C     *  OSIG       OIL SURFACE TENSION                           (DYNE/CM)
C
C     *  LINE 9.....(FOR IAT=1 AND IAT=3)...OIL FLUX.....................
C     *  QP         OIL FLUX FOR IAT = 1 CASES                     (M/D)
C     *  TPB        OIL EVENT BEGINNING TIME                        (D)
C     *  TPE        OIL EVENT ENDING TIME                           (D)
C     *  HS         CONSTANT HEAD FOR IAT=3 CASES                   (M)
C     *
C     *  LINE 9.....(FOR IAT = 2)...OIL VOLUME..........................
C     *  PVOL       OIL VOLUME/AREA INCORPORATED INTO THE SOIL      (M)
C     *  DPL        LOWER DEPTH OF INITIALLY POLLUTED ZONE          (M)
C     *
C     *  LINE 10....DISSOLVED CONSTITUENT...............................
C     *  COINI      INITIAL CONCENTRATION IN OIL (SEE NOTE 5.)    (MG/L)
C     *
C     *  LINE 11....DISSOLVED CONSTITUENT...............................
C     *  PARTITIONING COEFFICIENTS:
C     *  XXKO       OIL/WATER        (C0 = XXKW*CW)                 (*)
C     *  XXKV       OIL/AIR          (CA = XXKV*CO)                 (*)
C     *  XXKS       SOLID/WATER (CONSTITUENT)                      (L/KG)
C     *  XXKSH      SOLID/WATER (HYDROCARBON)                      (L/KG)
C     *  RHOS       BULK DENSITY OF MATRIX                        (GR/CC)
C     *
C     *  LINE 12....VOLATILIZATION MODEL................................
C     *  DAIR       DIFFUSION COEFFICIENT FOR CONSTITUENT IN AIR   (M2/D)
C     *  DWV        DIFFUSION COEFFICIENT FOR WATER VAPOR          (M2/D)
C     *  EVAP       WATER EVAPORATION RATE (VOL./AREA/TIME)        (M/D)
C     *  TEMP       TEMPERATURE                                     (C)
C     *  RH         RELATIVE HUMIDITY                               (*)
C     *
```

```
C     *  LINE 13....OILENS SUB-MODEL PARAMETERS (1).....................
C     *  RADI       SOURCE RADIUS                                    (M)
C     *  RMF        RADIUS MULTIPLYING FACTOR                        (*)
C     *  FRING      HEIGHT OF CAPILLARY FRINGE                       (M)
C     *  VDISP      VERTICAL DISPERSIVITY OF AQUIFER               (M2/D)
C     *  GRAD       GROUNDWATER GRADIENT                             (*)
C     *  SPRB       TRAPPED OIL SATURATION BELOW THE WATER TABLE     (*)
C     *
C     *  LINE 14....OILENS SUB-MODEL PARAMETERS (2).....................
C     *  SOLC       WATER SOLUBILITY OF CONSTITUENT                (MG/L)
C     *  SOLH       WATER SOLUBILITY OF HYDROCARBON (OIL)          (MG/L)
C     *
C     *  LINE 15....SIMULATION PARAMETERS...............................
C     *  TM         SIMULATION ENDING TIME   (SEE KSTOP)             (D)
C     *  DM         MAXIMUM SOLUTION TIME STEP                       (D)
C     *  DTPR       MINIMUM TIME BETWEEN PRINTED TIME STEPS AND      (D)
C     *             MASS BALANCE CHECKS
C     *  KSTOP      ENDING CRITERIA                                  (*)
C     *             1  USER SPECIFIED ENDING TIME (TM)
C     *             2  OIL LENS MOTION STOPS
C     *             3  CONSTITUENT MASS FLUX TO AQUIFER LESS THAN MAXIMUM
C     *             4  CONSTITUENT MASS IN OIL LENS LESS THAN OPERC*
C     *                MAXIMUM CUMULATIVE INFLUX TO LENS
C     *             (1 IS DEFAULT FOR NO OILENS SIMULATION OR WHEN OIL
C     *             DOES NOT REACH THE WATER TABLE BEFORE TIME = TM)
C     *  OPERC      FACTOR USED WITH KSTOP = 4  (0.0 < OPERC < 1.0)  (*)
C     *
C     *  LINE 16....PROFILES............................................
C     *  NTIMES     NUMBER OF PROFILES (UP TO 10)                    (*)
C     *
C     *  LINE 17........................................................
C     *  PR(NTIMES) PROFILE TIMES                                    (D)
C     *             OMIT LINE 17 IF NTIMES = 0
C     *
C     *  LINE 18....TSGPLUME INPUT PARAMETERS...........................
C     *  DLONG      AQUIFER LONGITUDINAL DISPERSIVITY                (M)
C     *  DTRAN      AQUIFER TRANSVERSE DISPERSIVITY                  (M)
C     *  PMAX       PERCENT OF MAXIMUM CONSTITUENT RADIUS            (*)
C     *  CMINW      MIMINUM RECEPTOR WELL CONCENTRATION OF INTEREST (MG/L)
C     *  NWELL      NUMBER OF RECEPTOR WELLS (UP TO 8)               (*)
C     *
C     *  LINE 19....TSGPLUME INPUT PARAMETERS 2..........................
C     *  BEGT       BEGINNING TIME                                   (D)
C     *  ENDT       ENDING TIME                                      (D)
C     *  TINC       TIME INCREMENT                                   (D)
C     *  TAQU       AQUIFER THICKNESS                                (M)
C     *
C     *  LINE 20........................................................
C     *  XWELL(I)   X-COORDINATE OF RECEPTOR WELL                    (M)
C     *  YWELL(I)   Y-COORDINATE OF RECEPTOR WELL                    (M)
C     *
C     ******************************************************************
```

Appendix 11 Direct Editing of HSSM-T Data Files

The required parameters for HSSM-T are listed in Table 115. As with HSSM-KO, all input data is format free. It is recommended to create new HSSM-T input data files by running HSSM-KO.

Table 115 HSSM-T Input Data File Structure

```
C     *****************************************************************
C     * TSGPLUME INPUT DATA
C     *
C     * LINE 1
C     *   IFILE    KOPT/OILENS INPUT DATA FILE (A40)
C     * LINE 2
C     *   OFILE    KOPT/OILENS OUTPUT DATA FILE (A40)
C     * LINE 3
C     *   TFILE    TSGPLUME INPUT DATA FILE (A40)
C     * LINE 4
C     *   KKSTOP   KOPT/OILENS STOPPING CRITERIA (A40)
C     * LINE 5
C     *   AL       LONGITUDINAL DISPERSIVITY (M)
C     *   AT       TRANSVERSE DISPERSIVITY (M)
C     *   AV       VERTICAL DISPERSIVITY (M)
C     *   VEL      SEEPAGE VELOCITY (M/D)
C     *   POR      POROSITY (*)
C     *   TAQU     AQUIFER THICKNESS (M)
C     * LINE 6
C     *   R        RETARDATION FACTOR (*)
C     *   PMAX     PERCENT MAXIMUM CONTAMINANT RADIUS (*)
C     *   CMIN     MINIMUM OUTPUT CONCENTRATION (MG/L)
C     *   ZLAM     AQUIFER DECAY COEFFICIENT (1/D)
C     * LINE 7
C     *   BTIME    BEGINNING TIME (D)
C     *   ETIME    ENDING TIME (D)
C     *   TINTE    TIME INCREMENT (D)
C     * LINE 8
C     *   NWELL    NUMBER OF RECEPTOR WELLS (*)
C     * LINE 9 TO 9 + NWELL-1
C     *   XX       X COORDINATE OF WELL (M)
C     *   XY       Y COORDINATE OF WELL (M)
C     * LINE 9 + NWELL TO END
C     *   TI       TIME (*)
C     *   RC       RADIUS OF CONTAMINANT (M)
C     *   HF       HYDROCARBON FLUX (KG/D)
C     *   CF       CONTAMINANT FLUX (KG/D)
C
C     *****************************************************************
```

Appendix 12 PRE-HSSM Input Data Templates

The following tables are to be used as input data templates for the MS-DOS version of HSSM. Each input data screen in PRE-HSSM is represented by a template. These pages are intended as aids for preparing input data sets.

Simulation Control Switches		
Variable	**Description**	**Value**
IFACE	Interface Flag	D
IWR	Print Flag	
IKOPT	KOPT Flag	
ICONC	Concentration Flag	
ILENS	OILENS Flag	
ITSGP	TSGPLUME Flag	

Output File Names		
File	**Description**	**Stem Name**
*.HSS	HSSM-KO Formatted Output File	
*.PL1	HSSM-KO Plot File 1	
*.PL2	HSSM-KO Plot File 2	
*.PL3	HSSM-KO Plot File 3	
*.PMI	HSSM-T Input Data File	
*.TSG	HSSM-T Formatted Output File	
*.PMP	HSSM-T Plot File	

Run Title

Matrix Properties

Variable	Description	Value
WKS	Saturated Hydraulic Conductivity (m/d)	
RKS	Ratio of Horizontal to Vertical Conductivity	
KRF	Relative Permeability Selection Index	
XLAMB	If KRF = 1 Brooks and Corey's Lambda If KRF = 2 van Genuchten's n	
ETA	Porosity	
SWR	Residual Water Saturation	

Hydrologic Properties

Variable	Description	Value
WMU	Dynamic Viscosity of Water (cp)	
WRHO	Density of Water (g/cm^3)	
IRT	Recharge Input type	
QW/SWMAX	If IRT = 1 Water Flux (m/d) If IRT = 2 Water Saturation	
XMKRW	Maximum Relative Permeability During Infiltration	
WTABLE	Depth to the Water Table (m)	

NAPL Phase Properties

Variable	Description	Value
PMU	NAPL Dynamic Viscosity (cp)	
PHRO	NAPL Density (g/cm^3)	
SPR	Vadose Zone NAPL Trapped Saturation (*)	
IAT	NAPL Application Type 1=flux specified 2=volume/area specified 3=constant head ponding 4= variable ponding after constant head period	

Capillary Suction Approximation Parameters

Variable	Description	Value
HWE	If KRF = 1 Brooks and Corey's Air Entry Head (m) If KRF = 2 van Genuchten's α (1/m)	
WSIG	Surface Tension of Water (dyne/cm)	
OSIG	Surface Tension of NAPL (dyne/cm)	

NAPL Flux Boundary Condition (IAT = 1)

Variable	Description	Value
QP	NAPL flux (m/d)	
TPB	NAPL Event Beginning Time (d)	
TPE	NAPL Event Ending Time (d)	

NAPL Volume/Area Boundary Condition (IAT = 2)

Variable	Description	Value
PVOL	NAPL Volume/Area (m)	
DPL	Lower Depth of the NAPL Zone (m)	

Constant NAPL Head or Variable Head Ponding (IAT = 3, 4)

Variable	Description	Value
TPB	NAPL Event Beginning Time (d)	
TPE	NAPL Event Ending Time (d)	
HS	Constant Head (m)	

Dissolved Constituent Concentration

Variable	Description	Value
COINI	Initial Concentration in NAPL (mg/l)	

Equilibrium Linear Partition Coefficients

Variable	Description	Value
XXKO	NAPL/Water	
XXKS	Chemical Consitutent Solid/Water (L/Kg)	
XXKSH	NAPL Solid/Water (L/Kg)	
RHOS	Bulk Density (g/cm^3)	

OILENS MODEL PARAMETERS: 1

Variable	Description	Value
RADI	Radius of the Source (m)	
RMF	Radius Multiplication Factor (*)	
FRING	Lens Spreading Parameter (m)	
VDISP	Vertical Dispersivity of Aquifer (m)	
VEL	Groundwater [Darcy] Velocity (m/d)	
SPRB	Aquifer Trapped NAPL Saturation (*)	

OILENS MODEL PARAMETERS: 2

Variable	Description	Value
XMSOL	Maximum NAPL Saturation in Lens	
SOLC	Constituent Water Solubility (mg/L)	
SOLH	Hydrocarbon (NAPL) Water Solubility (mg/L)	

Simulation Parameters

Variable	Description	Value
TM	Simulation Ending Time (d)	
DM	Maximum Solution Time Step (d)	
DTPR	Minimum Time Between Printed Time Steps (d)	
KSTOP	Ending Criterion	
OPERC	Mass Fraction (KSTOP = 4)	

Profiles

Variable	Description	Value
NTIMES	Number of Profile Times	

Profile Times

Variable	Description	Value
PR(1)	Profile Time (d)	
PR(2)	Profile Time (d)	
PR(3)	Profile Time (d)	
PR(4)	Profile Time (d)	
PR(5)	Profile Time (d)	
PR(6)	Profile Time (d)	
PR(7)	Profile Time (d)	
PR(8)	Profile Time (d)	
PR(9)	Profile Time (d)	
PR(10)	Profile Time (d)	

TSGPLUME Data

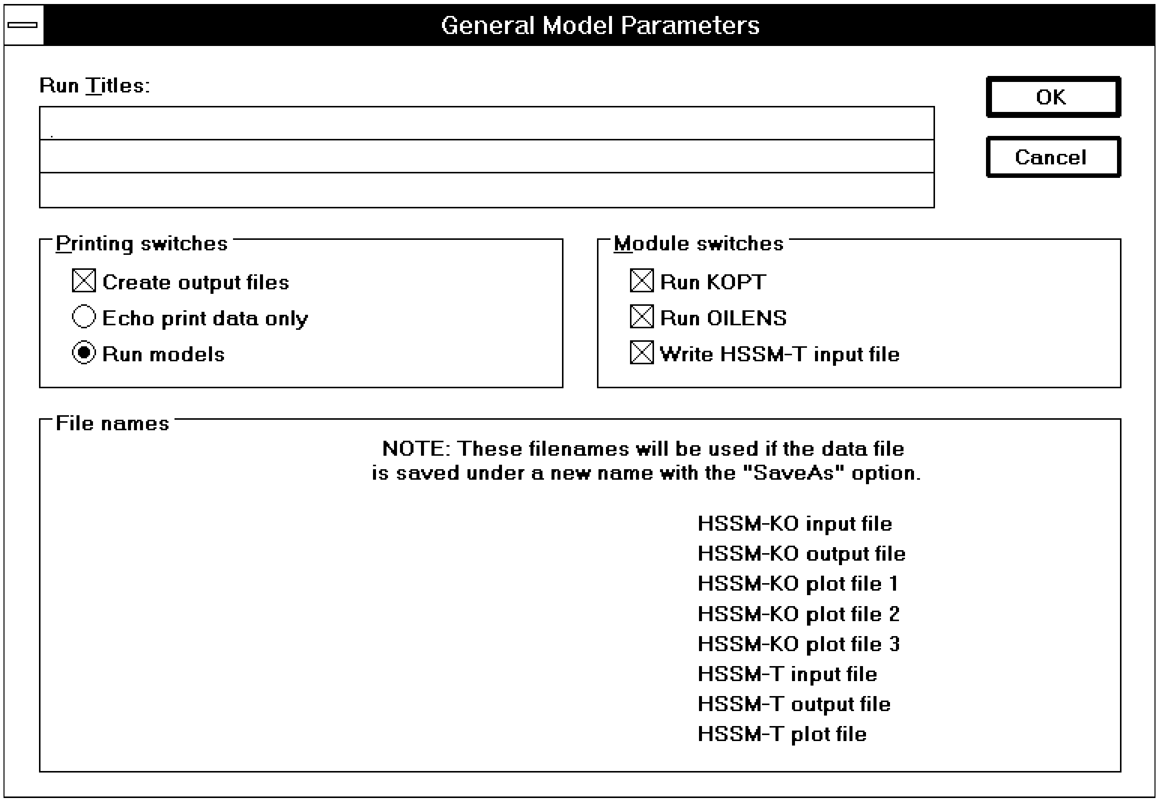
Variable	Description	Value
DLONG	Aquifer Longitudinal Dispersivity (m)	
DTRANS	Aquifer Transverse Dispersivity (m)	
PMAX	Percent Maximum Contaminant Radius	
CMINW	Minimum Output Concentration (mg/L)	
ZLAM	Aquifer Decay Rate Coefficient (1/d)	
NWELL	Number of Receptor Points	

TSGPLUME Simulation Times		
Variable	**Description**	**Value**
BEGT	Beginning Time (d)	
ENDT	Ending Time (d)	
TINC	Time Increment (d)	
TAQU	Aquifer Thickness (m)	

Receptor Well Locations			
Variable	**Description**	**X Value**	**Y Value**
X(1), Y(1)	X and Y Coordinates of Receptor 1		
X(2), Y(2)	X and Y Coordinates of Receptor 2		
X(3), Y(3)	X and Y Coordinates of Receptor 3		
X(4), Y(4)	X and Y Coordinates of Receptor 4		
X(5), Y(5)	X and Y Coordinates of Receptor 5		
X(6), Y(6)	X and Y Coordinates of Receptor 6		

Appendix 13 HSSM-WIN Input Data Templates

The following figures are to be used as input data templates for the MS-Windows interface (HSSM-WIN). Each input dialog box in HSSM-WIN is represented by a template. These pages are intended as aids in preparing input data sets.



Printing switches

☒ Create output files

○ Echo print data only

● Run models

Module switches

☒ Run KOPT

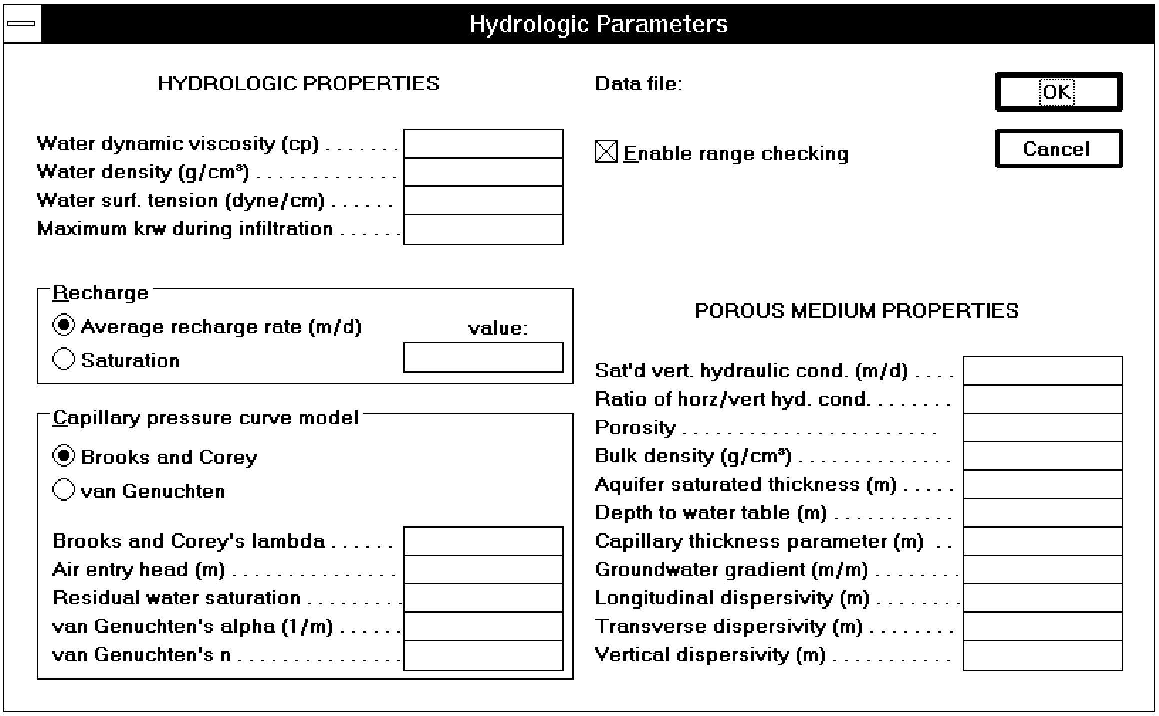
☒ Run OILENS

☒ Write HSSM-T input file

File names

NOTE: These filenames will be used if the data file is saved under a new name with the "SaveAs" option.

HSSM-KO input file
HSSM-KO output file
HSSM-KO plot file 1
HSSM-KO plot file 2
HSSM-KO plot file 3
HSSM-T input file
HSSM-T output file
HSSM-T plot file



Hydrologic Parameters

HYDROLOGIC PROPERTIES

Water dynamic viscosity (cp) . . . .
Water density (g/cm³) . . . .
Water surf. tension (dyne/cm) . . . . . .
Maximum krw during infiltration . . . . . .

Recharge
● Average recharge rate (m/d)
○ Saturation
value:

Capillary pressure curve model
● Brooks and Corey
○ van Genuchten

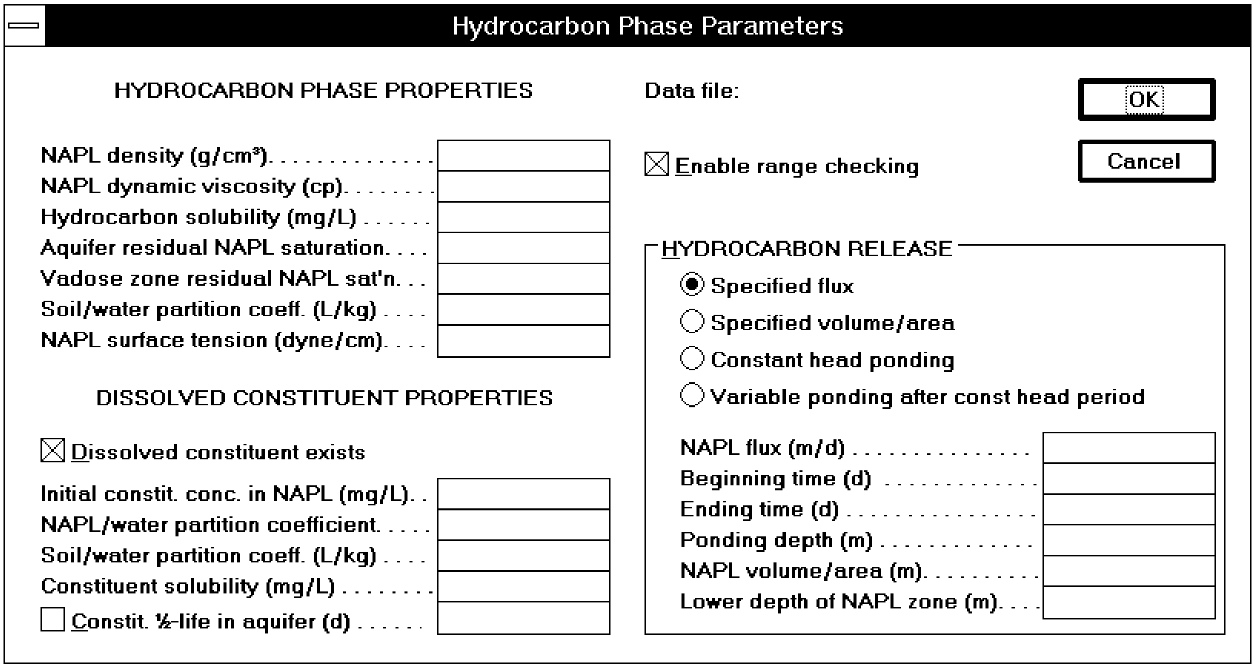
Brooks and Corey's lambda . . . . . .
Air entry head (m) . . . .
Residual water saturation . . . .
van Genuchten's alpha (1/m) . . . . . .
van Genuchten's n . . . .

Data file:

☒ Enable range checking

POROUS MEDIUM PROPERTIES

Sat'd vert. hydraulic cond. (m/d) . . . .
Ratio of horz/vert hyd. cond. . . . .
Porosity . . . .
Bulk density (g/cm³) . . . .
Aquifer saturated thickness (m) . . . . .
Depth to water table (m) . . . .
Capillary thickness parameter (m) . .
Groundwater gradient (m/m) . . . .
Longitudinal dispersivity (m) . . . .
Transverse dispersivity (m) . . . .
Vertical dispersivity (m) . . . .



Hydrocarbon Phase Parameters

HYDROCARBON PHASE PROPERTIES

NAPL density (g/cm^3). . . . .
NAPL dynamic viscosity (cp). . . . .
Hydrocarbon solubility (mg/L) . . . . . .
Aquifer residual NAPL saturation. . . .
Vadose zone residual NAPL sat'n. . .
Soil/water partition coeff. (L/kg) . . . .
NAPL surface tension (dyne/cm). . . .

DISSOLVED CONSTITUENT PROPERTIES

☒ Dissolved constituent exists

Initial constit. conc. in NAPL (mg/L). .
NAPL/water partition coefficient. . . . .
Soil/water partition coeff. (L/kg) . . . .
Constituent solubility (mg/L) . . . .
☐ Constit. ½-life in aquifer (d) . . . . . .

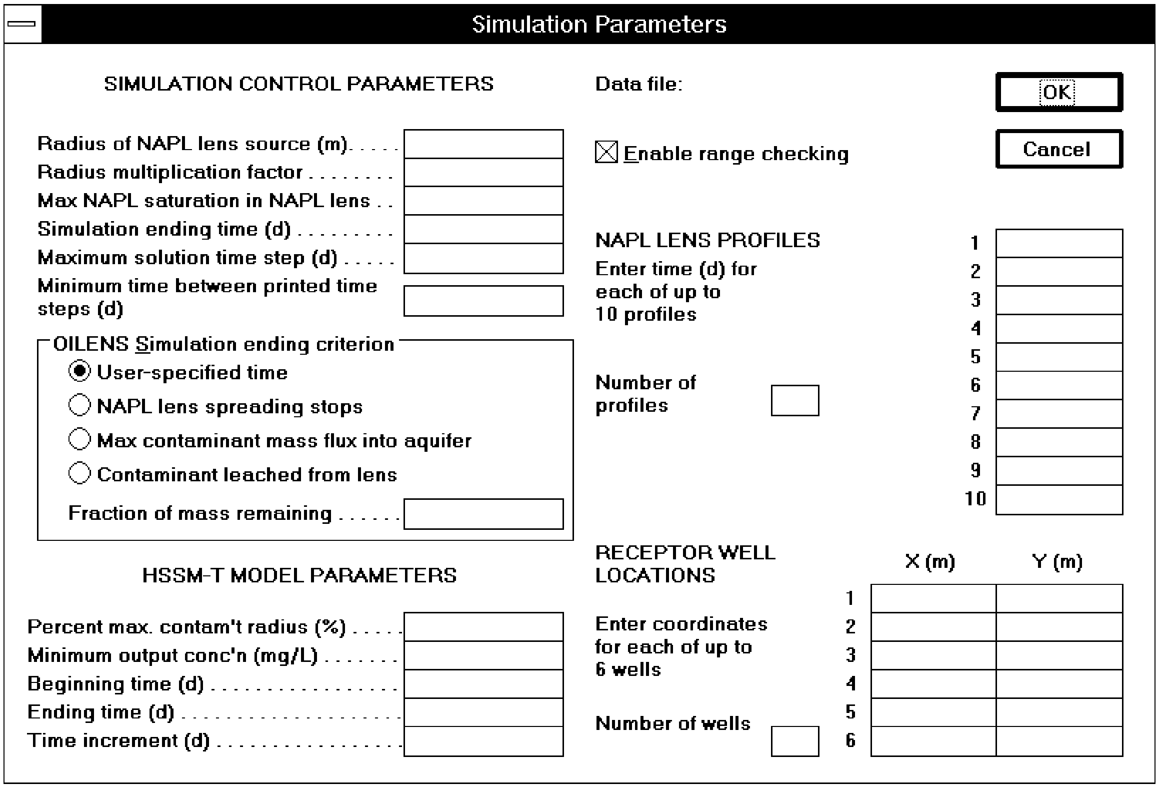
Data file:

☒ Enable range checking

HYDROCARBON RELEASE

- ● Specified flux
- ○ Specified volume/area
- ○ Constant head ponding
- ○ Variable ponding after const head period

NAPL flux (m/d) . . . .
Beginning time (d) . . . .
Ending time (d) . . . .
Ponding depth (m) . . . .
NAPL volume/area (m). . . . .
Lower depth of NAPL zone (m). . . .



Simulation Parameters

SIMULATION CONTROL PARAMETERS

Radius of NAPL lens source (m). . . . .

Radius multiplication factor . . . .

Max NAPL saturation in NAPL lens . .

Simulation ending time (d) . . . .

Maximum solution time step (d) . . . . .

Minimum time between printed time steps (d)

OILENS Simulation ending criterion

● User-specified time

○ NAPL lens spreading stops

○ Max contaminant mass flux into aquifer

○ Contaminant leached from lens

Fraction of mass remaining . . . . . .

HSSM-T MODEL PARAMETERS

Percent max. contam't radius (%) . . . . .

Minimum output conc'n (mg/L) . . . .

Beginning time (d) . . . .

Ending time (d) . . . .

Time increment (d) . . . .

Data file:

☒ Enable range checking

NAPL LENS PROFILES

Enter time (d) for each of up to 10 profiles

1	
2	
3	
4	
5	
6	
7	
8	
9	
10	

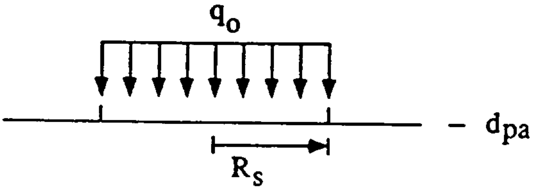
Number of profiles

RECEPTOR WELL LOCATIONS

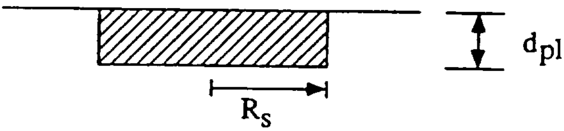
Enter coordinates for each of up to 6 wells

	X (m)	Y (m)
1		
2		
3		
4		
5		
6		

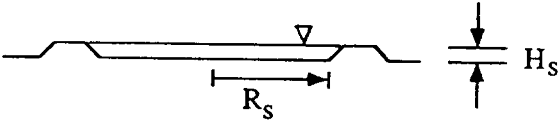
Number of wells



1. Flux Source Representation



2. Volume Source Representation



3. Constant Head Source Representation

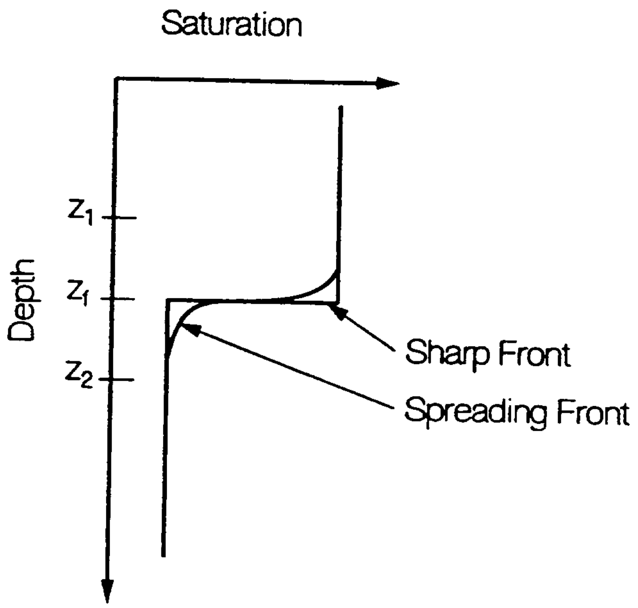


Figure 5 Comparison of sharp and spreading fronts

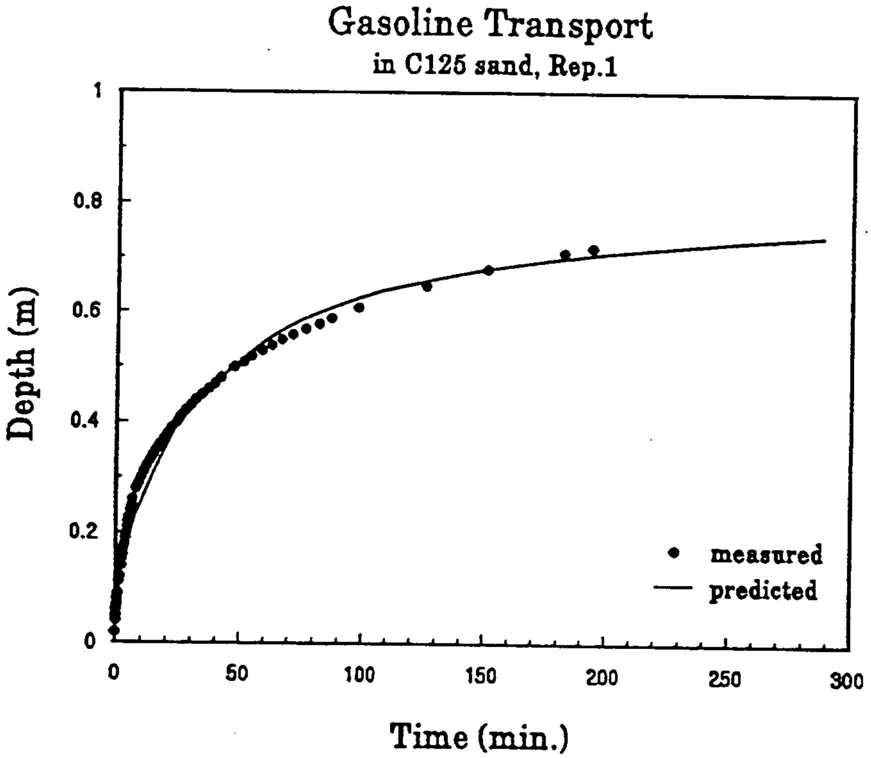


Figure 6 Comparison between experimental data and the KOPT model

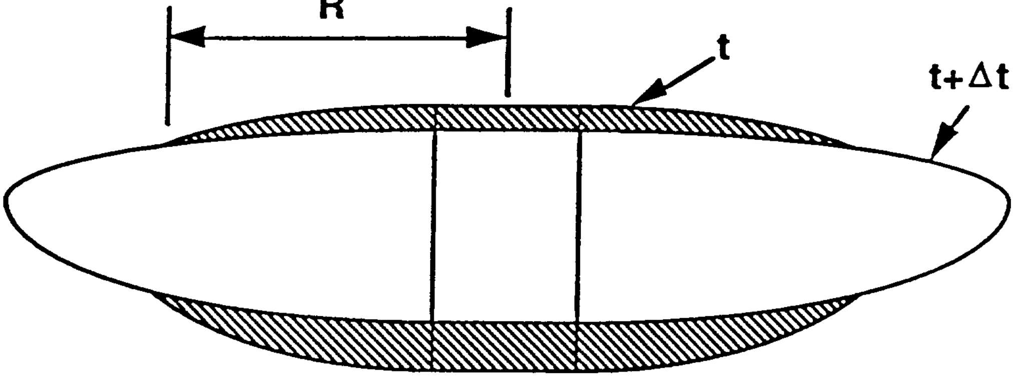


Figure 7 Lens configuration during thinning phase

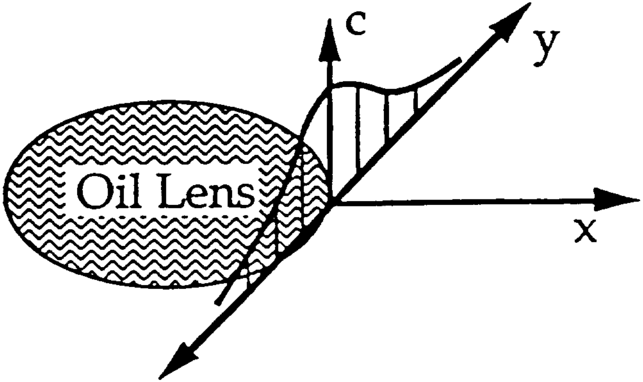


Figure 8 Gaussian source configuration used in TSGPLUME

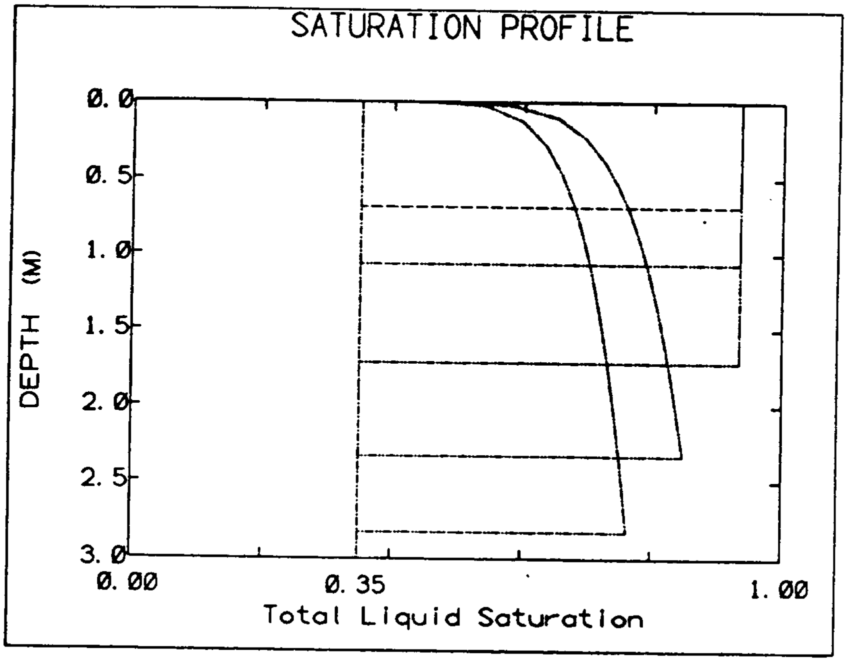


Figure 40 Saturation profiles

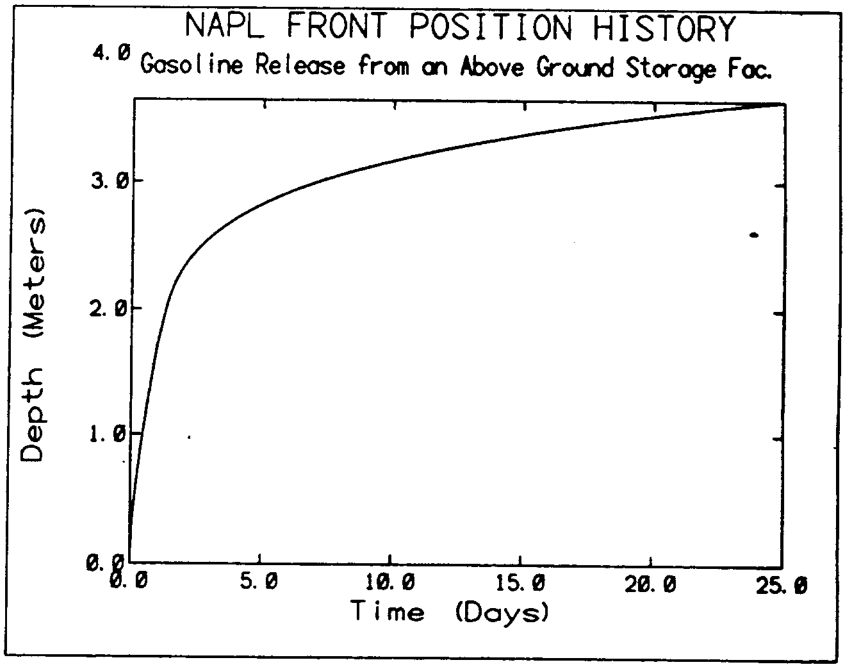


Figure 41 The front position

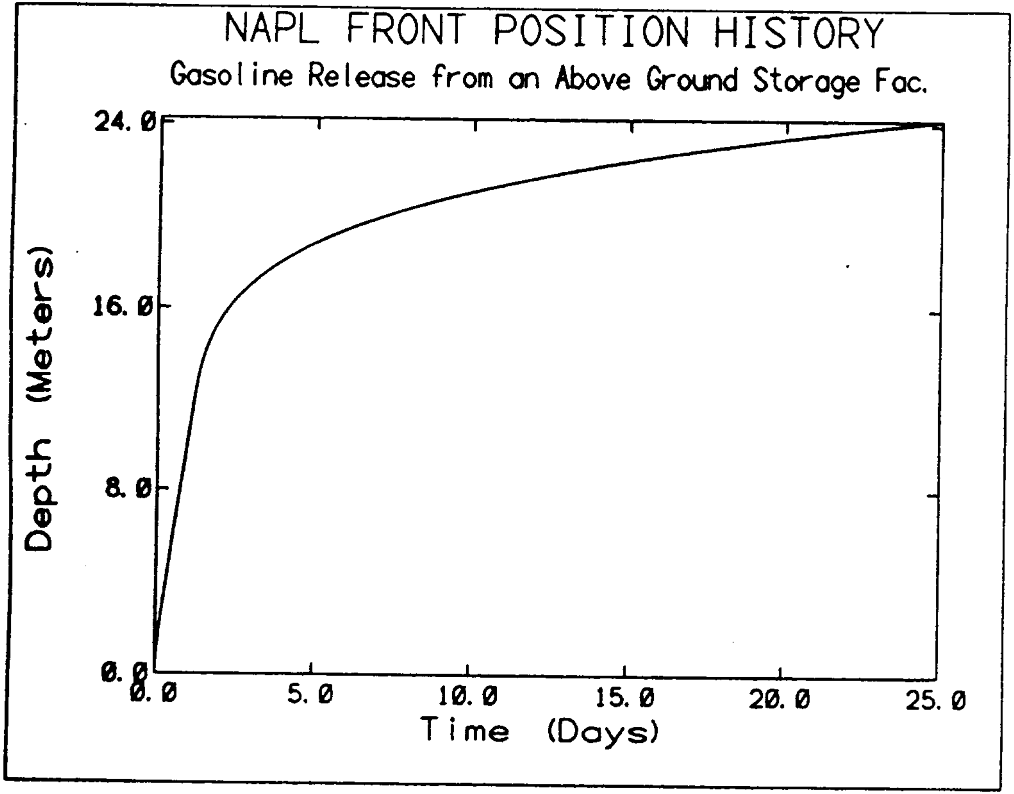


Figure 42 Storage tank facility example with increased conductivity